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Research Articles

THE DIAGNOSTICS POSSIBILITIES OF ANAEROBIC POWER AND CAPACITY BY USING THE PEDAR SYSTEM

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Abstract

The aim of this study was to evaluate the possibilities of execution of the 60 second Bosco test of anaerobic power and capacity using the Emed system with mobile pedographic system Pedar in field conditions. Apart from evaluating the common parameters of maximal anaerobic power and anaerobic capacity of an individual using the above mentioned system, we also focused on differences in the variables of each limb. The system Emed with mobile pedographic facility Pedar is possible to be used for the diagnostics of anaerobic power and capacity evaluated by Bosco test in field conditions. We did not notice any statistically important difference in aerial and contact phase of the dominant and non-dominant limb during the 60 seconds of the test while observing the signs of domination of the limbs. Therefore there were not any signs of domination of the limbs.

Keywords

Anaerobic power and capacity; Bosco test; Pressure distribution measurement.

Introduction

In the last 50 years, the level of aerobic (oxidative) power and capacity defined by the maximal consumption of oxygen and the derived parameters and their diagnostics have been standardized and the tests of measuring the aerobic power and capacity are generally recognized [11]. Under the terms of secular trends amongst the population, only some of the norms and specifications of the predictive equation containing particular components of aerobic capability [9] appear to be a matter of revision. The aerobic capabilities influencing the endurance performance are an important part of the battery for evaluating the health-orientated capability of the individual as a factor influencing the health in a significant way.

However, there is a different situation with anaerobic abilities. In the general approach towards the problematic of anaerobic abilities and their diagnostics, there are still persisting problems and doubts [3]. The processes as well as the mechanisms of the anaerobic way of releasing the energy in the bone muscle at the activities of the maximal and submaximal intensity are diagnostically rarely available, therefore it is possible to encounter a wide range of conceptions and methodological solutions which always accent some and also suppress other aspects of the anaerobic metabolism [6]. There is no generally accepted parameter for evaluating the level of anaerobic power and capacity. The maximum values of the afterload blood lactate are often used for evaluating the anaerobic capacity despite of problems with the interpretation of the physiological meaning [4].

Tests of anaerobic abilities are missed out while evaluating the health-orientated capability for complicated interpretation of the health impact on as wide a range as possible of age categories. Currently they are appearing as a possible component of test batteries evaluating the general level of health-orientated capability. Ortega et al. [10] observes the validity and reliability of the test for the determination of the health-orientated capability, beside other things, also for the determination of anaerobic abilities. Čaba [2] proved close connection between the output in Bosco test and the items of the test battery Eurofit, describing the power endurance parameters of the lower limb such as long jump from standing, sit up, and endurance running in adolescents. From the results of Bosco test it is partly possible to predict a specific level of health-orientated capability in adolescents.

In the diagnostics of the prerequisite for short term highly intense activity performed in the conditions of oxygen deficit, there are used anaerobic load tests which track the changes of the performance in time. It means that they register not only the maximal anaerobic lactate performance but also the decrease in the performance during the test. A separate category of the anaerobic capability tests is a test of repetitive jumps. Bosco test of repetitive jumps [1] enables the determination of anaerobic capacity by defining the height of the jumps and anaerobic performance in the test. The way of the execution of the test doesn't represent any risk of complicated execution and termination of the test (in comparison with other anaerobic tests, i.e., the Kindermann-Schnabel one). The content of the test is performing of all series of the consequential repetitive vertical jumps, as maximal as possible, in the time period of 60 seconds. The performance in the jump phase of the jump test in first 15 seconds shows close connection towards the representation of fast muscle fibre [5].

The test is usually executed in a lab on the jump ergometer which enables to evaluate the overall number of jumps (spring), the average time of one jump (s), absolute work (kJ), and relative work (J/kg).

The system Emed with foot pressure inset Pedar (Novell, Germany) is a modern system for measuring the distribution of the pressure and local load under the sole, between the foot and the shoe, in static and dynamic conditions. It enables both lab and also field testing during natural activities such as walking, running, bike riding, therefore the results are more relevant in real life. It also enables to diagnose not only the data expressing the plantar pressure but also to diversify while in contact with the mat between the eccentric and concentric phase. The eccentric component in vertical jump includes the impact on the mat and retaining the potential energy by the extensors of lower limbs. The concentric phase generates the power from the chemo-mechanical conversion of the energy and the utilization of saved elastic energy for the spring [9].

1 Aim of the Research

The goal of this project was to evaluate the possibilities of execution of the 60 second Bosco test of the anaerobic capabilities using the Emed system with mobile pedographic Pedar system in field conditions. Apart from evaluating the common parameters of maximal anaerobic power and the capacity of the individual using the above mentioned system, we focused on the differences of the variables of particular limbs.

2 Methodology

The measurement was taken in a test group of 18 men participants. Because of incorrect performing of the test, the results of three participants were excluded, and the results of another person were excluded because of not finishing the load test. The basic anthropometric characteristics of the assessed individuals are shown in Tab. 1.

Tab. 1: *Basic characteristic of tested people (arithmetic mean ± SD)*

Quantity	Age [years]	Weight [kg]	Height [m]	Laterality LL left	Laterality LL right
14	21.2±1.1	74.1±8.4	1.81±0.05	6	8

LL – lower limb
Source: Own research

The physical height was measured in a straighten-up position without shoes using the altimeter Anthropometer A 213 (Trystom spol. s.r.o., Czech Republic) with the accuracy 0.1 cm. The physical weight was measured on the personal scales Amboss©Seca 899 (Hamburg, Germany) with the accuracy 0.1 kg.

For the load test we used the 60 second Bosco test of repetitive jumps [1]. Its content is the series of consequential repetitive maximal vertical jumps in 60 seconds.

The evaluated variables were the capacity in the test and the overall work as an indicator of anaerobic capacity, jump height, time of the aerial phase (Tf) and their summarization in the time period of 60 seconds, and the contact phase (Tc). We observed the signs of tiredness determined as the index evaluated by the decrease of performance in a time. The variables Tf and Tc were evaluated together for both limbs and also separately for each limb afterwards.

The tested participants stretched before performing the test. The test itself was started from the position of a squat, the angle under the knee was 90°, arms akimbo. We watched the technique of performing the test as well as the angle in the knee which was not allowed to be less than 90°. The testing took place in the sports hall on artificial surface.

For measuring of the powers impacting the mat we used the Emed system with the foot pressure inset Pedar (Pedar-x; Novel, Munich, Germany), which was placed directly into the shoe of the tested person. The frequency of the recorded dynamic parameters was 100 Hz.

In the third and the fifth minute after the test the measurement of the afterload concentration of lactate (la) in the blood was taken by the Lactate meter HP-Cosmos Sirius (HP Cosmos©, Germany).

Determination of the dominance of lower limbs was done by the performance test on stairs. We monitored which limb would be in dominant position, e.g. which limb would be used first by the tested person for stair climbing and descending. The laterality had already been verified before the test, observing the dominant limb in participants kicking a ball.

For the statistic processing of the research data we used the method of descriptive and inductive statistics. The data were processed in the Excel program.

3 Results

The measured data in Bosco test were split into 6 intervals of 10 seconds each. In these intervals we set the number of jumps and the time of contact with the inset. Other counted variables were based on the following formulas [1]:

$$v = 0.5 \times g \times T_f \quad (1)$$

v – speed of take off [m.s^{-1}], where T_f is the time of aeriel phase and g is the constant of acceleration.

$$h = 0.125 \times g \times {T_f}^2 \quad (2)$$

h – jump height [m].

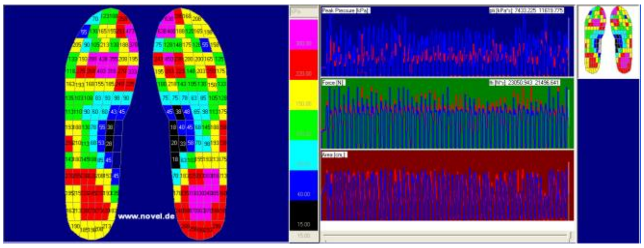
$$A = m \times g \times h = 0.125 \times g^2 \times {T_f}^2 \times m \tag{3}$$

A – work [J], where m is the weight of the tested individual [kg].

$$IU = (work\ max - work\ min) \tag{4}$$

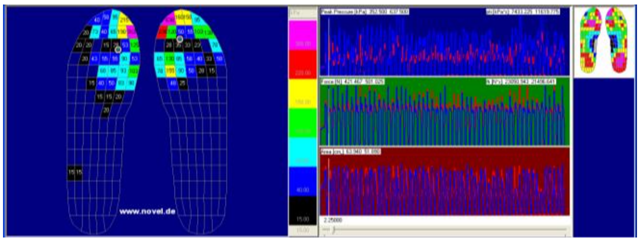
IU – Fatigue index.

The example of the record and graphic processing of the data Novel is shown in Fig. 1 for the landing phase. Fig. 2 shows the contact with the inset after the phase of taking off and leaving the inset.



Source: Own research

Fig. 1: *An example of the record and graphic processing of data using the Pedar system while landing on the inset*



Source: Own research

Fig. 2: *An example of record and graphic processing of the data using the Pedar system after the take off phase and leaving the inset*

The general results of Bosco test for both limbs together are shown in Tab. 2.

Tab. 2: *The results of Bosco test (arithmetic mean ±SD)*

Person	Number of jumps	Contact phase [s]	Aerial phase [s]	Speed of take off [m.s^{-1}] average	Jump height [m]	Jump height average [m]	Work [J]	Fatigue index
1	53	36.96 (±0.05)	26.78 (±0.03)	2.51 (±0.16)	14.08 (±0.32)	0.27 (±0.32)	11281.24 (±28.26)	841.59 (±93.9)
2	55	39.25 (±0.04)	20.77 (±0.04)	1.85 (±0.21)	9.68 (±0.04)	0.18 (±0.04)	8066.89 (±32.17)	471.88 (±26.63)
3	68	32.45 (±0.03)	27.55 (±0.03)	1.99 (±0.13)	13.78 (±0.03)	0.2 (±0.03)	8511.65 (±16.64)	260.3 (±13.86)
4	46.5	40.27 (±0.09)	19.73 (±0.07)	2.08 (±0.32)	8.43 (±0.05)	0.18 (±0.05)	4876.88 (±28.25)	508.64 (±34.14)
5	62.5	34.4 (±0.08)	25.6 (±0.09)	2.01 (±0.45)	13.17 (±0.08)	0.21 (±0.08)	9298.26 (±57.56)	916.38 (±62.89)
6	72	43.34 (±0.13)	16.66 (±0.06)	1.13 (±0.3)	5.71 (±0.04)	0.08 (±0.04)	4812.86 (±34.08)	759.95 (±48.8)
7	49	41.43 (±0.15)	18.57 (±0.08)	1.86 (±0.38)	8.97 (±0.08)	0.18 (±0.08)	6600.68 (±49.02)	722.67 (±88.12)
8	80.5	21.26 (±0.03)	38.74 (±0.05)	2.36 (±0.25)	22.84 (±0.05)	0.28 (±0.05)	15005.38 (±35.47)	1091.2 (±44.7)
9	56	40.48 (±0.23)	19.52 (±0.1)	1.71 (±0.51)	10.5 (±0.13)	0.19 (±0.13)	8750.07 (±106.51)	2981.64 (±547.56)
10	69	29.17 (±0.05)	30.83 (±0.06)	2.19 (±0.27)	17.04 (±0.05)	0.25 (±0.05)	13370.9 (±40.9)	1017.42 (±46.62)
11	54	33.61 (±0.07)	26.39 (±0.07)	2.4 (±0.32)	15.91 (±0.07)	0.29 (±0.07)	1248.1 (±54.48)	1050.46 (±64.6)
12	47	41.51 (±0.14)	18.49 (±0.07)	1.93 (±0.33)	8.84 (±0.05)	0.19 (±0.05)	6070.56 (±36.48)	702.69 (±56.52)
13	61	36.31 (±0.05)	23.69 (±0.05)	1.9 (±0.22)	11.38 (±0.04)	0.19 (±0.04)	7590.15 (±27.3)	381.08 (±25.07)
14	60	33.54 (±0.06)	26.46 (±0.05)	2.16 (±0.23)	14.28 (±0.05)	0.24 (±0.05)	9384.57 (±31.08)	770.28 (±54.97)

Source: Own research

The majority of the tested people are based on Heller and Vodička [7] recreational sportspeople who show the values of the aerial phase around 36.6 s and the contact phase 23.4 seconds. With ranking into this category corresponded also the average values of afterload lactate, which were on the level 7.8 ± 2.6 mmol/l at the 3rd minute and on the level 8.9 ± 1.9 mmol/l at the 5th minute. The tested people were mainly present in the zones of anaerobic lactate load.

The values of the variable T_c fluctuated between 21.26 s and 43.34 s. At the lower values of the contact phase we can find higher number of jumps (correlation coefficient r = –0.73, where the indirect high dependence is $0.90 > r \geq 0.70$).

The lowest values of the contact phase were noticed from its beginning until 20 seconds in the test. With coming tiredness the values were increasing. The values of variables T_f fluctuated between 16.66 s and 30.83 s. While watching the relationship of variable number of jumps and the aerial phase we noticed middle (significant) dependence (r = 0.64).

While watching the signs of domination of the limbs in the test, we didn't notice any statistically significant differences in the aerial phase at the dominant and non-dominant limb during the 60 seconds of the test, not even in the closing part of the test, where tiredness can usually be observed. The average values of the differences at variables in the aerial and the contact phase are shown in Tab. 3.

Tab. 3: *Average values of the difference T_f and T_c – the lower limbs*

Intervals 10s	**1.**	**2.**	**3.**	**4.**	**5.**	**6.**
T_c [s]	0.00	0.00	–0.01	0.00	0.00	–0.01
T_f [s]	–0.02	–0.02	–0.03	–0.02	–0.02	–0.03

Source: Own research

Conclusion

The system Emed with pedographic facility Pedar is possible to be used in diagnostics of anaerobic power and capacity evaluated by the Bosco test in field conditions. The hypothesis number 1 was confirmed. Apart from the evaluated variables, where it is possible to get the usual jump ergonometric, such as the maximal anaerobic power and the capacity of the individual, it is possible to evaluate, thanks to the above-mentioned system, the detailed distribution of the pressure on the sole and e.g. the technique of performing the takeoff from the whole foot or its upper part. The advantage of this system is the possibility of its transportation and usage in field conditions and on different surfaces.

While watching the signs of domination of the limbs in the tests, we did not notice any statistically significant differences in the aerial phase at the dominant and non-dominant limb during the 60 seconds of the test, not even in the closing part of the test, where tiredness can usually be observed. We did not confirm the hypothesis number 2 which assumes the higher tiredness sign at the non-dominant limb evaluated with prolonging the contact phase and shortening the aerial phase.

Acknowledgements

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MOŽNOSTI DIAGNOSTIKY ANAEROBNÍCH SCHOPNOSTÍ SYSTÉMEM PEDAR

Cílem projektu bylo zhodnotit možnosti provedení 60ti sekundového Boscova testu anaerobních schopností pomocí systému Emed s mobilním pedografickým systémem Pedar v terénních podmínkách. Kromě vyhodnocení běžných parametrů maximálního anaerobního výkonu a anaerobní kapacity jedince pomocí uvedeného systému jsme se zaměřili na rozdíly v proměnných u jednotlivých končetin. Systém Emed s mobilním pedografickým zařízením Pedar lze využít k diagnostice anaerobních schopností hodnocených Boscovým testem v terénních podmínkách. Při sledování projevu dominance končetin během testu jsme nezaznamenali statisticky významné rozdíly v letové a kontaktní fázi u dominantní a nedominantní končetiny během 60 sekund trvání testu, nedošlo tedy k projevům dominance končetin.

MÖGLICHKEITEN DER DIAGNOSTIZIERUNG VON ANAEROBEN FÄHIGKEITEN MIT DEM SYSTEM PEDAR

Ziel des Projekts war, die Möglichkeiten der Durchführung des sechzig Sekunden dauernden Bosco-Test anaerober Fähigkeiten mit Hilfe des Systems Emed mit dem mobilen pedografischen System Pedar unter Geländebedingungen zu bewerten. Außer der Bewertung der gängigen Parameter der maximalen anaeroben Leistung und der anaeroben Kapazität des Einzelnen mit Hilfe des angeführten Systems konzentrieren wir uns auf die Unterschiede in den veränderlichen Werten der einzelnen Gliedmaßen. Das System Emed mit der mobilen pedografischen Anlage Pedar ist einsetzbar zur Diagnostik anaerober Fähigkeiten, die mit dem Bosco-Test unter Geländebedingungen bewertet wurden. Bei der Beobachtung dieses Dominanzausdrucks während des Tests haben wir keine statistisch relevanten Unterschiede in der Flug- und Kontaktphase bei den dominanten und nicht dominanten Extremitäten während des sechzig Sekunden dauernden Tests vermerkt. Es gab also keine Anzeichen von Dominanz der Extremitäten.

MOŻLIWOŚCI BADANIA WYDOLNOŚCI BEZTLENOWEJ PRZY WYORZYSTANIU SYSTEMU PEDAR

Celem projektu była ocena możliwości przeprowadzenia 60-sekundowego Testu Bosco wydolności beztlenowej przy pomocy systemu Emed z mobilnym systemem pedograficznym Pedar w warunkach terenowych. Oprócz badania zwykłych parametrów maksymalnej mocy anaerobowej przy pomocy ww. systemu skupiono się na różnicach w zmiennych dotyczących poszczególnych kończyn. System Emed z mobilnym urządzeniem pedograficznym Pedar można wykorzystać do diagnozowania wydolności beztlenowej przy pomocy Testu Bosco w warunkach terenowych. Obserwując przejawy dominacji kończyn podczas testu nie odnotowano podczas 60 sekund trwania testu statystycznie istotnych różnic w fazie lotu i kontaktu z podłożem w przypadku kończyny dominującej i niedominującej, co oznacza brak pojawienia się dominacji kończyn.

SPRINGS CONNECT PEOPLE AND LANDSCAPES – ENVIRONMENTAL EDUCATION AND COOPERATION IN THE REGION LIBEREC-ZITTAU

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Abstract

This paper describes the trilateral transboundary project Prameny spojují/Quellen verbinden launched in 2016 under the coordination of the Technical University of Liberec. The aim of the project is a complex hydrochemical, hydrobiological, hydrological, geological and human geographical assessment of a set of about 40 springs in the region Liberec – Zittau through educational and research networking of the partner universities. This region has considerably humid climatic environment reflected in a high number of springs, whose mutual multidisciplinary assessment has been largely missing. Preliminary example results at the Ploučnice spring reveal a calcium-bicarbonate water originating from the Bohemian Cretaceous Basin, with slightly elevated spring values of Cd and autumn values of Pb in the sediment. The spring ecosystem is characterized by seminature montane mixed forest, with presence of freshwater shrimp in the spring water. The Ploučnice spring is one of the most abundant springs in Central Europe with a good water quality, which has promoted the use of this water for drinking purposes around 1900, and until the 1960’s for water energy in the nearby mills.

Keywords

Education; Environmental sciences; Springs; Chemistry; Biology; Transboundary region.

Introduction

Water has a vital importance for mankind; although it is a renewable resource, it is necessary to protect it and sustainably manage its use. Special attention should be given to possible sources of drinking water, namely groundwater and its surface discharges – springs. Hydrochemical analysis of spring water and in sediment delivers information about the quality of spring water and its interaction with surrounding rocks and soils. Studying biota in springs and their surroundings reveals the relations between water and living organisms in headwater areas. Finally, exploring the relationship of man to springs at his living place describes cultural aspects linked with the importance of water.

Focused on above mentioned topics, the project *Prameny spojují/Quellen verbinden* has been created by researchers from the Technical University of Liberec, Czech University of Life Sciences and Technical University of Dresden in 2016. This three-year project aims to improve the skills of students of participating universities, to promote international research cooperation and implement educational activities. Hydrochemical, hydrobiological, hydrological and human geographical research of springs is an important instrument to achieve its objectives.

The abundant surface water and groundwater resources in the region Liberec-Zittau and its surroundings have been recently addressed by several transboundary projects [1], [2], [3]. These studies have dominantly addressed the groundwater and surface water hydrology and/or their links to the land use and human activities. A complex hydrochemical, hydrobiological, hydrological, geological and human geographical assessment at the transboundary scale has not yet been performed.

4 Research Aim and Objectives

This project is based on an assessment of about 40 selected springs in the transboundary Liberec-Zittau area. They were selected upon relevant available information and field pre-screening of about 100 springs, which represent the variety of geological, hydrochemical, hydrological, hydrobiological and human geographical aspects of the study area. During the first project year, a research methodology was created and first results have been obtained. This paper presents the adopted methodology (Fig. 1) and addresses the preliminary results on the example of the Ploučnice spring. It is expected that this methodology will serve to future assessment of further springs in this area and also complement the environmental education in the transboundary region Liberec-Zittau. Complete results will be published at the project end in 2019.

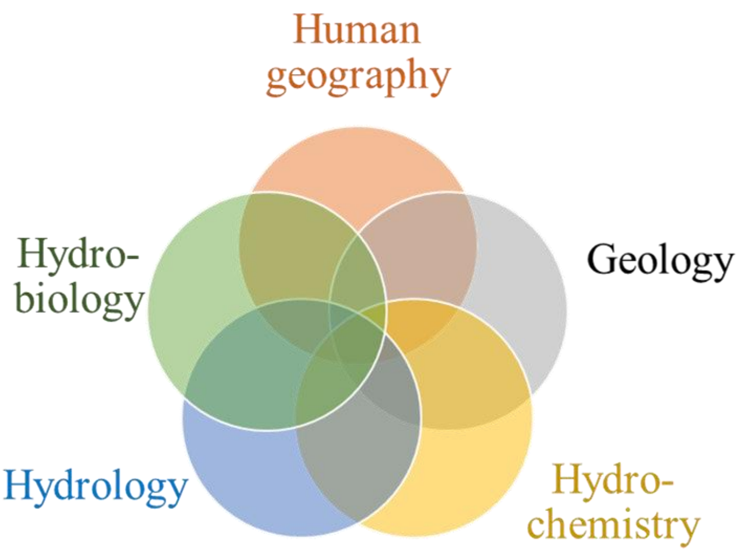

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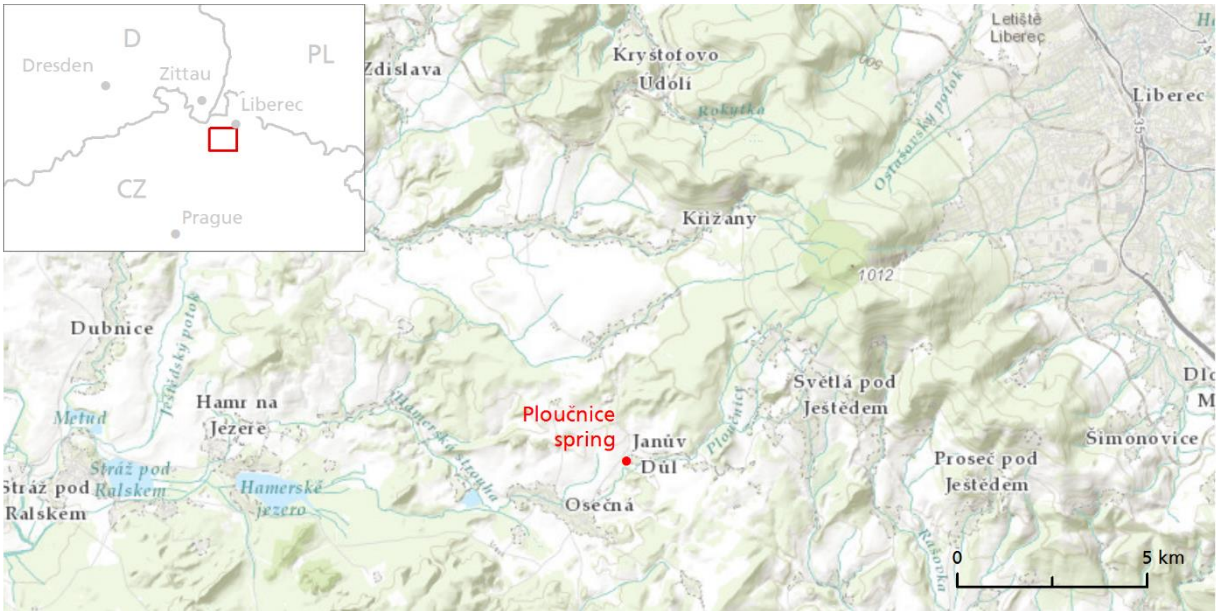
Fig. 3: *Scheme of the methodology of the project Prameny spojují/Quellen verbinden*

1 Materials and Methods

1.1 Overview of the Area

The project study area (Fig. 2) covers the transboundary zone on the borders between Czech Republic and Germany (Saxony). It is located in the districts Liberec, Ústí n.L. and Görlitz approximately between the cities of Liberec, Zittau, Rumburk, Nový Bor, Český Dub and Turnov. The area largely belongs to the Western Sudetes geomorphological region (in Czech: Krkonošská oblast, in German: Westsudeten) with major ranges Jizera Mountains (Jizerské hory – Isergebirge), Lusatian Mountains (Lužické hory – Lausitzer Gebirge) with the Saxonian part Zittau Mountains (Zittauer Gebirge), Lusatian Hills (Šluknovská pahorkatina – Lausitzer Bergland), Ještěd-Kozákov-Ridge (Ještědsko-Kozákovský hřbet – Jeschken-Kosakow-Kamm), and major sedimentary basins around Liberec and Zittau: the multilayered Bohemian Cretaceous Basin (Česká křídová pánev – Böhmisches Kreidebecken) and tertiary Zittau Basin (Žitavská pánev – Zittauer Becken). The area is traversed by the main European water divide between the Baltic Sea and Northern Sea watersheds and drained by major rivers Neisse, Mandau and Ploučnice. The climate of the area includes temperate and cold humid types with increased continentalism in the Zittau and Bohemian Cretaceous Basins. The long-term annual precipitation amount varies between approximately 1400 mm in the higher elevations of the mountains and 640 mm in the lowlands, with precipitation maxima in July and August [2]. High intense rainfall occurs frequently during spring and summer. The Jizera Mountains are characterized by snow cover lasting up to 160 days/year. The mean annual temperature varies between 8 °C in the lowlands and 5 °C in the mountains [4]. The all-time maximum daily precipitation amount at the territory of the Czech Republic (345 mm) was measured in the central part of the Jizera Mountains.



Source: Own data, basemap: ESRI

Fig. 4: *Location of Ploučnice spring within the transboundary study area*

The complex geological structure of the area is dominated by granites and granodiorites in the Jizera Mountains, by basaltoid volcanic in the Lusatian Mountains and Lusatian Hills, by metamorphic rocks of Ještěd-Kozákov-Ridge, by sandstones in the Zittau Mountains, and by Cretaceous sandstones to claystones in the Bohemian Cretaceous Basin. The crystalline and sedimentary formations are divided by the Lusatian fault. Basaltic and phonolitic hilltops are mostly present in the western part, whereas the lowlands in the Zittau and Liberec basins are dominated by Quaternary loess. Major aquifers in the area with extended stream-aquifer communication are formed in Cretaceous sandstones southbound from the Lusatian fault. These aquifers consist of a lower Cenomanian layer with overlying layers from Turonian and Coniacian age [5].

The soils have a range of properties, particularly with respect to runoff formation, erosion, solute transport and water storage capacity [6]. While the soils on mountainous hill slopes are mostly shallow, often skeleton-rich dystric cambisols, podzols and leptosols with low storage capacities, the valleys are filled by organosols that release humic and fulvic acids. The agricultural soils are mostly luvisols and stagnic luvisols with a high silt content and a low infiltration rate. They are partly affected by poorly drained horizons. Luvisols are easily erodible and contribute to the suspended load in the rivers. The lowland flood plains are typically covered by gleysols [2]. The land use differs according to the soil types. While the mountainous areas are dominated by spruce forests, the fertile soils in the lowlands are agriculturally exploited. Substantial parts of the Jizera Mountains and Lusatian Mountains in the Czech Republic as well as the Zittau Mountains in Germany were declared as nature protection zones.

1.2 Flora and Fauna

Vegetation characteristics of the spring surroundings were described using two methods: biotope description and fytocenological relevés. In the field, the main biotope types were identified in a circle of about $100 m^2$ that was delimited around the spring [7]. The dominant plant species in the identified biotopes were determined in each vegetation layer (tree, shrub and herb layers). The tree individuals were also recorded. The identified semi-natural types of biotopes became subject of a more detailed characteristic, using the fytocenological relevés approach (Br. – Bl. scale, [8]). This approach determines the type of vegetation using the fytocenological system. The vegetation type will serve for evaluation of the anthropogenic influence to spring surroundings.

Benthic invertebrates represent the most important animals in springs. Whereas meiofauna (benthic animals under 0.5 mm) is observable by a microscope only, macroinvertebrates (benthic animals above 0.5 mm [9]) are visible to the naked eye and can be observed by a visitor of a spring. Considering the aim of the project, macroinvertebrates were selected as the organisms group representing a biota of the studied springs.

Macroinvertebrate samples were collected twice a year by a quantitative method. A perpendicularly embed plastic tube (diameter of 12 cm, length of 20 cm) was used for a demarcation and a cutting out of a representative spring bottom area. A surface layer of sediment was mined from the tube using a small ladle. A volume of a subsample was 400 cm^3 of the bottom sediment. Six of such subsamples were carried out at every sampling date, covering different types of the bottom of the spring (mud, sand, gravel, organic sediments). These 6 subsamples were merged into one sample, representing one spring at one date.

Yet in field, the sample was sieved over a net of 0.5 mm to eliminate a fine substrate and reduce the sample volume. The sample was then placed in shallow bowls. Visible invertebrates were selected, saved in a small separate container and fixed by 70% ethanol. Only flatworms (Turbellaria) were saved alive in a small amount of spring water, because their determination needs a native form. All the remained material was saved in 1 l plastic containers and preserved by 70% ethanol.

In the CULS laboratory, samples were sorted using a stereomicroscope. Macroinvertebrates unnoticed in the field were selected and main taxonomical groups and species were determined.

1.3 Chemistry

Water samples for hydrochemical analysis were collected approximately once a month in 250ml plastic bottles (PE) – one for cations, one for anions and one for bicarbonate titration. On-site pH-value and dissolved oxygen and electrical conductivity (EC) were measured using a Multimeter (WTW Multi 3430). Redox-potential was measured by a WTW pH 320. Where possible, discharge of the spring was measured by the "Bucket and Stopwatch method" [10].

Water samples were analysed in the TUD-IHI laboratory in Zittau for major ions (NO_3^-, SO_4^{2-}, Cl^-, PO_4^{3-}) by Ion Chromatograph (Dionex ICS-1100) and selected elements (e.g. Ca, Mg, Fe, Al, K, U, As) by inductively coupled plasma with optical emission spectrometry (ICP-OES, PerkinElmer) according to DIN EN ISO 11885 (www.iso.org), and inductively coupled plasma mass spectrometry (ICP-MS, PerkinElmer) according to DIN EN ISO 17294-2 (www.iso.org) depending on their concentration. Bicarbonate concentration was carried out using titration with HCl.

The data interpretation was carried out using software package Diagrammes [11]. The interpretation included the control of the ionic balance (equal sum of major anions and cations), determination of hydrochemical water types and data plotting in the form of particular hydrochemical plots.

The sampling of sediment in the springs was carried out twice a year (spring, autumn). Sediment samples were collected in plastic containers and frozen upon the return to laboratory. In the laboratory, the seamples were further processed by lyophilisation (freeze-drying), homogenisation, sieving and microwave decomposition. After the decomposition the concentrations of metals in the samples were analyzed in the CULS laboratory by use of spectrometers FAAS a GTAAS (Agilent Technologies).

1.4 Human Geography and GIS

The human geographic dimension of the assessment of springs deserves attention since springs have been used by people for several reasons: (1) spring water has been used for drinking and cattle and plant watering; (2) people took care of the springs since they were sources of drinking water; (3) springs were used as meeting places; (4) water from particular springs was sometimes believed to have a healing effect.

In the presented project, springs are evaluated from the human geography perspective based on their use in selected historical eras: (1) industrialization of the Liberec-Zittau region until 1918; (2) era between 1918 and 1945; (3) period immediately after the expulsion of Sudeten Germans; (4) era of collectivisation (1950s); (5) era of mass suburbanization (1990s); (6) current era. There is an assumption that after 1945 the usage of springs changed significantly because of the expulsion of German population from the most of the Czech part of the selected territory and resettlement of the Czech population from inland. Consequently, also the toponymy and local names changed significantly, especially after 1945. In some cases, there was only a translation of the original German name to Czech, in others, new original Czech names were created or the newcomers brought the toponymy with them from their original homes. Toponymy is a constituent part of the cultural landscape since it is an expression of the creation of identities [12]. For this reason, the analysis of toponymy is an additional part of the springs' research. In addition to the official place names also local names, names used by the local residents themselves, are also subjects of the analysis. They are collected and examined using the method of mental mapping in particular, where the specific local names are identified by local population on the large-scale maps.

The primary method of the data collecting for the analysis of springs forming the human geography perspective is semi-structured interviewing. It means that the interview schedule is prepared with fully worded questions, but the respondents are given enough space to explain their stances and postures freely [13]. During the first round of interviews, the mayors of selected villages of particular interest were interviewed. The method of semi-structured interviewing was combined with oral history [14], aimed at identifying the stories and legends connected to the springs. The major effort in this research phase is to find witnesses of different historical eras with the aim to find out how the springs were used in a defined time period and to collect various stories and legends particular springs are surrounded by. Based on these findings it is possible to identify the local identities which have been created thanks to collective memory and shared meaning of a place or genius loci [15]. Springs became part of the local legends and fairy tales; sometimes they are connected to the existence of supernatural beings and rituals such as "opening of the wells".

These primary methods are complemented by the archival research of historical documents and analysis of old maps, since there is an assumption that if the springs are located on old maps they were widely used in the past. Therefore, the basic objective of this method is to identify the existing springs on the old maps with the critical evaluation of the particular sources and the historical era they were produced in.

Several GIS-based tools are being prepared within the framework of the project. A prominent example is the simplified geological map 1:100.000 covering both the Czech and German parts of the study area. The map was constructed using ArcGIS on the ESRI basemap platform from the following sources: mainly geological map of Czech 1:50 000 from geology.cz (http://mapy.geology.cz/geocr_50/), detailed Geological Map of the area Lausitz-Jizera-Karkonosze, and German geological map (Geologische Übersichtskarte der Bundesrepublik Deutschland 1:200.000 (GÜK200) – CC 5550 Görlitz).

2 Results and Discussion

This chapter describes preliminary results on the example of the Ploučnice spring (Fig. 3).

The Ploučnice spring is one of the best-known springs in the Podještědí (Lower Ještěd) region. It has already been marked on old maps, such as on the map sheet Turnov of the historical mapping of 1951. Its original name in German language was "Polzenquelle" and the current name "Pramen Ploučnice" is a literal translation from German. An interesting fact is that this spring, called "Pramen Ploučnice" is not the real source of the river Ploučnice, but it got its name because of its largest discharge level (Interview with the mayor of Janův Důl, Jan Mašek, 26. 7. 2016). The spring has a form of a small lake with several groundwater inflows (Fig. 3).

Source: Photo by M. Kändler

Fig. 5: *Photo of the Ploučnice spring (June 22nd 2016)*

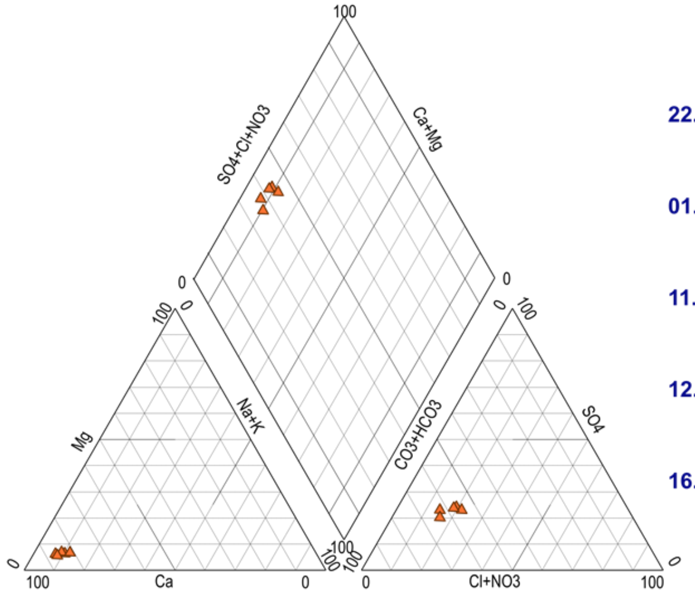
The Ploučnice spring is situated in the Bohemian Cretaceous Basin, in the valley between Osečná and Janův Důl. Majority of the area around the valley is covered by marine sand to fine grained conglomerate consisting of small clasts of quartz of Turonian age belonging to Jizera Formation. The sand is partially lithified, partially cross-bedded, indicating the high energy sedimentation environment. However, the valley itself is filled by quaternary sediments, mainly loess from last glacial period (Upper Pleistocene) with intercalations of fine quartz clasts and with carbonate filling. The place surrounding the spring is formed by sub recent (quaternary) fluvial clay, sand and gravel. The whole area is fragile, deformed from northeast to southwest direction, which is indicated by short tectonic faults. Part of the faults was rejuvenated during Tertiary (Eocene to Oligocene) and filled by dispersed alkaline volcanic veins. The nearest basaltoid vent is situated about 1 km southwest from the Ploučnice spring [5].

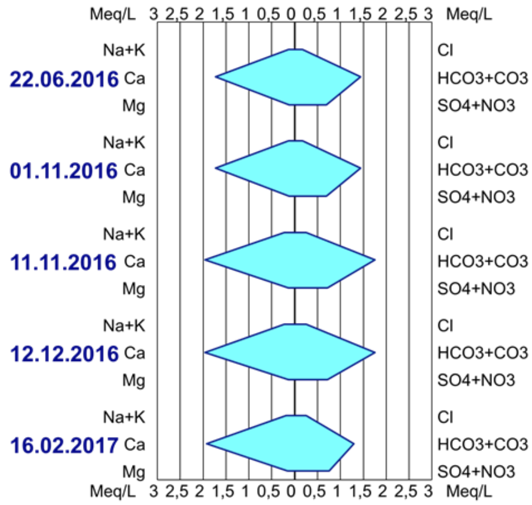
The vegetation around the Ploučnice spring is characterized by a seminatural mixed montane sycamore-beech forest with dominant *Acer pseudoplatanus*, *Fagus sylvatica* and sporadically mixed with *Alnus incana*. The scrub layer is almost missing, whereas the herb layer is dominated by forest species such as *Athyrium filix-femina*, *Dryopteris filix-mas*, *Festuca altissima*, *Galium odoratum*, *Gymnocarpium dryopteris*, *Mercurialis perennis*, *Oxalis acetosella* and *Vaccinium myrthillus*. The character of the vegetation reveals a low human influence and almost no anthropogenic pollution of the closest spring surroundings.

Freshwater shrimp (*Gammarus fossarum*) was the absolutely most abundant macroinvertebrate species across the observed set of 40 localities, including the Ploučnice spring. In some springs, this animal represented over 90% of the sampled individuals. It is in accord with a wide occurrence of this species and its high ecological adaptability [16]. This species belongs to a typical spring fauna; however, generally it inhabits a large scale of running waters.

The second most abundant group of organisms Caddisflies (*Trichoptera*) also represents a common spring taxa. Stoneflies (*Plecoptera*) occurred in a lesser extent. However, one season is too short for an evaluation of occurrence of these animal groups; more comprehensive results are expected upon the complete 3-year survey.

Fig. 4 shows the concentrations of major ions (NO_3^-, SO_4^{2-}, Cl^-, HCO_3^-, Ca^{2+}, Mg^{2+}, Na^+, K^+) in sample water during five sampling turns at the Ploučnice spring in 2016/2017. This water has a rather moderate mineralization (average conductivity is 242 µS/cm), revealing water-rock interactions of the spring water prior to emerging on the surface. The average pH is 7.21 and the average dissolved oxygen concentration is 8.6 mg/l. The Piper and Stiff diagrams on Fig. 4 demonstrates that the dominant cation is Ca^{2+} and the dominant anion is HCO3-. Less abundant cation is the sum of Na^+ and K^+ and the less abundant anion is SO_4^{2-}. Mg^{2+} and the sum of NO_3^- and Cl^- are present only marginally. This is a typical pristine water type originating in carbonate rocks, with potential of drinking water use.

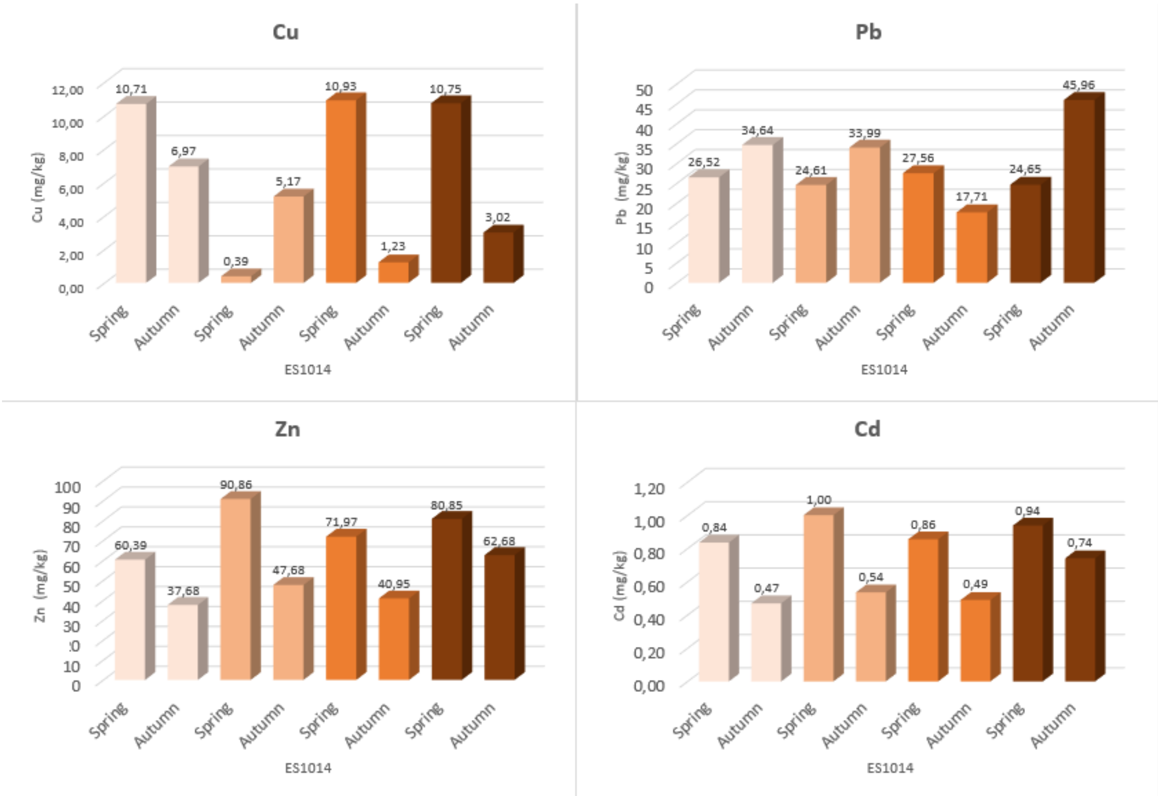




Source: Diagrammes software [9], own data

Fig. 6: *Piper (left) and Stiff diagrams (right) of 5 water samples from the Ploučnice spring*

Fig. 5 shows the concentrations of four toxic metals in the sediment of the Ploučnice spring, analysed in four sediment fractions (≤0.061 mm, 0.061-0.206 mm, 0.206-0.609 mm and >0.609 mm). Whereas Cu, Zn, and Cd showed higher concentrations in the spring period samples, the Pb concentrations were higher in the autumn. The spring concentration of Cd are very close to the environmental quality standard (EQS) of the USEPA (0.99 $mg \cdot kg^{-1}$). The measured higher autumn concentration of Pb in the fraction >0.609 mm have exceeded the EQS of USEPA (35.8 $mg \cdot kg^{-1}$). The concentrations of Zn and Cu remained below the EQS.



Source: Own data

Fig. 7: *Concentrations of selected metals (Cu, Pb, Zn, Cd) in the sediment of the Ploučnice spring. Results in the fractions ≤0.061 mm, 0.061-0.206 mm, 0.206-0.609 mm, and >0.609 mm are depicted.*

The Ploučnice spring has been widely used in the past. Nowadays, it is an interesting tourist point in this area. In the historical era, until approximately 1955 the Ploučnice spring was used to energy production because of its high level of discharge. There were many water mills built and during industrialization some of these mills were rebuilt to water turbines. One of the most important mills which were built nearby the spring is Jenišovský mill. After finishing the production of water energy from the spring, there was an intent to use the water form spring for production of soda water. This plan was, however, has been rejected by the local people since they were afraid that collection of water for this purpose would cause its scarcity [19]. An additional way of using the water from the Ploučnice spring was the creation of water supply around 1900. It consisted of a wooden pipe leading to the square where people used to scoop water from the fountain. These water pipes were not cleaned and maintained later so the usage of this water supply came to an end [19]. Currently, the water from spring is not being used for any purpose but the spring itself is maintained by the municipality of Osečná.

The Ploučnice spring is riddled with several legends. Some of them are based on the belief in the existence of supernatural beings; others are connected to the character of the spring itself. Probably the best-known of them, and mentioned in both interviews used in this brief study is a legend about the peasant who drove up to the spring with horses harnessed to a fully loaded carriage; and since the spring was very deep he got drown in it [19], [20]. Besides this legend, the respondents also mentioned the story about two children who wanted to swim in the spring but got drown because they did not estimate the depth of the spring properly, and the water was too cold [19], [20].

Concerning the supernatural beings, there is a vast amount of legends about watermen living by the spring. According to one of them, for example, there was a wicked waterman who drowned everybody who tried to poach in his water [17]. Another set of legends tells the stories about will-o'-the-wisps that attracted pilgrims to the water. Will-o'-the-wisps, however, are not only portrayed negatively, they also saved the life of one peasant by taking him out of the woods [18].

Conclusion

The project *Prameny spojují/Quellen verbinden* has accumulated a considerable amount of data from all participating disciplines, revealing a potential of a complex interdisciplinary assessment of this type of water resource at the transboundary scale. The survey of assessed 40 springs showed that water, sediment and biota in the spring ecosystems in the target region reflect a variety of geological, hydrochemical and hydrobiological settings as well as cultural and historical patterns. The field research on the springs will continue over this year, complementing the preliminary results from the last year and also including assessment of some new springs that have been pre-screened to potentially deliver useful information for all participating disciplines.

Acknowledgements

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PRAMENY SPOJUJÍ KRAJINY A STÁTY – ENVIRONMENTÁLNÍ VZDĚLÁVÁNÍ A KOOPERACE V REGIONU LIBEREC-ZITTAU

Tento článek popisuje trojstranný přeshraniční project Prameny spojují/Quellen verbinden, zahájený v roce 2016 a koordinovaný Technickou univerzitou v Liberci. Záměrem projektu je komplexní hydrochemické, hydrobiologické, hydrologické, geologické a humánně geografické zhodnocení souboru asi 40 pramenů v oblasti Liberec-Zittau, a to cestou vzdělávací a výzkumné spolupráce partnerských univerzit. Vlhké podnebí této oblasti se promítá do značného množství pramenů, jejichž společné multidisciplinární hodnocení nebylo dosud provedeno. Předběžné výsledky na příkladě pramenu Ploučnice ukazují vápenato-hydrogenuhličitanovou vodu pocházející z České křídové pánve, přičemž v pramenném ekosystému jsou přítomny sladkovodní různonožci. Pramen Ploučnice je jeden z nejvydatnějších pramenů ve střední Evropě s dobrou kvalitou vody, což kolem roku 1900 podporovalo její využití jako pitnou vodu a do 60. let minulého století využití jako vodní energii pro blízké mlýny.

QUELLEN VERBINDEN LANDSCHAFTSEINHEITEN UND STAATEN – UMWELTBILDUNG UND KOOPERATION IN DER REGION LIBEREC-ZITTAU

Dieser Artikel beschreibt das im Jahre 2016 begonnene und durch die Technische Universität Liberec koordinierte trilaterale grenzüberschreitende Projekt Prameny spojují/Quellen verbinden. Das Ziel des Projektes ist eine komplexe hydrochemische, hydrobiologische, hydrologische, geologische und humangeographische Beurteilung von ungefähr 40 Quellen in der Region Liberec-Zittau durch Bildungs- und Forschungskooperation der Partneruniversitäten. Diese Region ist durch ein feuchtes Klima mit zahlreichen Quellen charakterisiert, deren gemeinsame multidisziplinäre Betrachtung bisher nicht durchgeführt wurde. Vorläufige Ergebnisse am Beispiel der Ploučnice-Quelle zeigen auf ein Kalzium-Hydrogenkarbonathaltiges Wasser des Böhmischen Kreidebeckens, mit Vorkommen von Süßwasserkrebsen in dem Quellökosystem. Die Ploučnice-Quelle gehört zu den ergiebigsten Quellen Mitteleuropas mit guter Wasserqualität; dies führte um 1900 zur Nutzung als Trinkwasser sowie bis in die 60er Jahre des 20. Jahrhunderts zur Nutzung als Wasserenergie für die naheliegenden Mühlen.

ŹRÓDŁA ŁĄCZĄ REGIONY I KRAJE – EDUKACJA ŚRODOWISKOWA I KOOPERACJA W REGIONIE LIBEREC-ZITTAU

Niniejszy artykuł opisuje rozpoczęty w 2016 roku trójstronny transgraniczny projekt pn. Prameny spojují/ Źródła łączą, koordynowany przez Uniwersytet Techniczny w Libercu. Przedmiotem projektu jest kompleksowe hydrochemiczne, hydrobiologiczne, hydrologiczne, geologiczne i antropogeograficzne zbadanie około 40 źródeł znajdujących się w regionie Liberec-Zittau, realizowane w ramach współpracy uniwersytetów partnerskichw zakresie edukacji i badań naukowych. Region ten charakteryzuje się wilgotnym klimatem z licznymi źródłami, które do tej pory nie zostały jeszcze poddane wspólnym wielodyscyplinarnym badaniom. Wstępne wyniki, na przykładzie źródła Ploučnicy, wskazują na obecność wody wapienno-węglowodanowo-węglanowej pochodzącej z Czeskiej Niecki Kredowej, przy czym w źródliskowym ekosystemie występują obunogi słodkowodne. Źródło Ploučnicy zalicza się do najbardziej wydajnych źródeł w Europie środkowej charakteryzując się dobrą jakością wody; co doprowadziło około roku 1900 do jego wykorzystania jako źródła wody pitnej, a do lat 60. XX wieku do produkcji energii w okolicznych młynach.

THE ISSUE OF ENERGY RESOURCES IN THE PODKRUŠNOHOŘÍ REGION

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Abstract

Coal mining has had demonstrable negative impacts on the region and the landscape. In accordance with a growing number of inhabitants, the demand for energy consumption is constantly increasing. For the future, it is important to focus primarily on renewable energy resources, which will ensure the sustainable development of the environment and society. This contribution deals with the area in the Czech Republic that has had the greatest problems in this regard, namely North Bohemia (the Chomutov, Most, Teplice, and Ústí nad Labem districts). This is an area with significant anthropogenic activity, particularly due to the intensive mining of brown coal and in relation to the power industry. The Podkrušnohoří region has recently seen the partial suspension of mining limits at the Bílina Quarry, which is the reason why the regeneration of the region through reclamation and restoration will be needed. At the same time, this contribution contains a proposal for a possible change in the power industry, i.e. regarding the sources of renewable energy in the Podkrušnohoří region that could potentially be utilized after mining in individual quarries ends after 2050.

Keywords

Sustainable development; Renewable energy resources; Coal mining; North Bohemia.

Introduction

The Faculty of the Environment (the team from the Department of Natural Sciences) at the Jan Evangelista Purkyně University in Ústí nad Labem has been dealing with the issue of the anthropogenic burden on various regions after brown coal mining since 1992. It has collaborated on the region's regeneration with project architects, restoration company workers, mining company technicians, and farm managers. Their most important collaboration has been with Mostecká Uhelná Společnost [Most Coal Company] (now Czech Coal, a.s.), whereby research was carried out in the Slatenice, Pařidelský Lalok, Czechoslovak Army Quarry and Střimice dumps. Another place that has been and still is the focus of attention is the Radovesická dump in the Teplice district, whose area makes it the largest external dump in the Czech Republic.

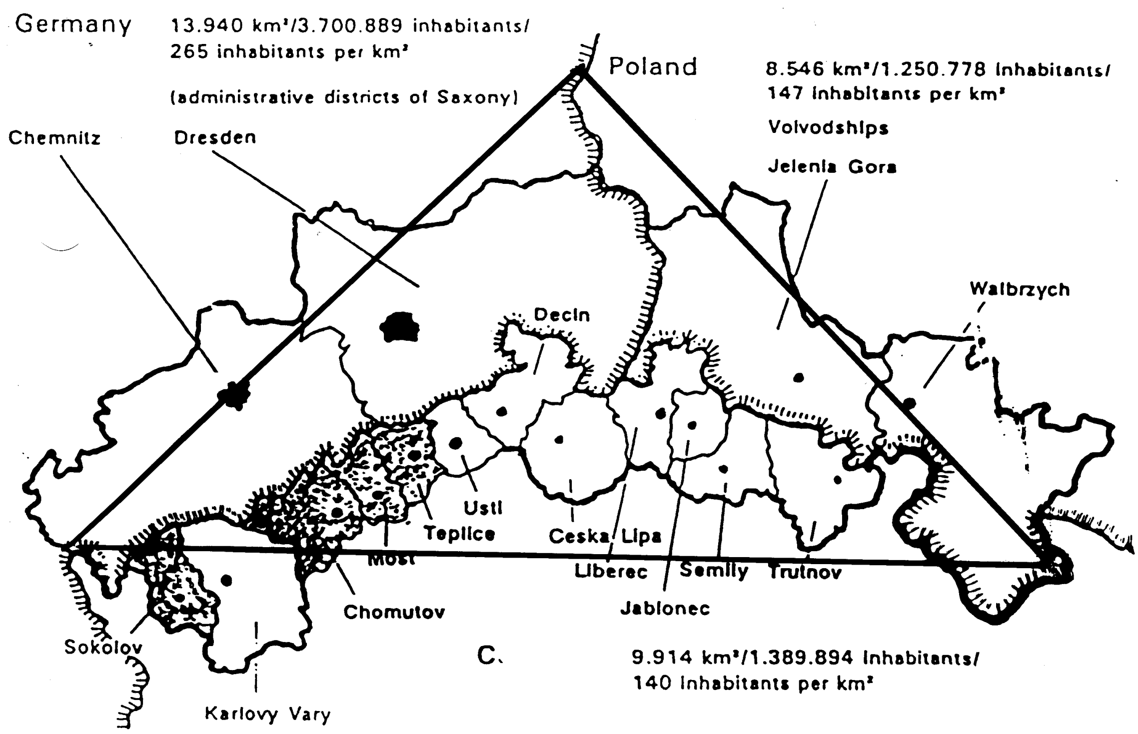
This research focused mainly on various forms of regeneration and individual types of restoration; a method called the Managed Succession of Localities after Mining in the Most Region was proposed, subsequently examined and evaluated. The issue of cultivating power-producing plants at the dumps was also addressed. For example, in 2007-2011, the aforementioned activities received support from the Ministry for Regional Development of the Czech Republic under project WD 44-07-1, "Model Solution for the Revitalization of Industrial Regions and Zones after Coal Mining, Using the Example of the Podkrušnohoří Region". The project's objective was to prepare an analysis of the main problems in the

Podkrušnohoří region and to study factors that disrupt the environment, such as the development of air quality, mining environment factors, disparities in the Land Fund, evaluation of recultivation in the area of interest, and other areas. The project resulted in proposals for sustainable management in the region and in the preparation and subsequent certification of the Revitalization Methodology in the Podkrušnohoří region.

At present, the theme of the revitalization of an anthropogenically affected region is being addressed within the scope of project No. QJ1520307, titled "Sustainable Forms of Management in an Anthropogenically Burdened Region". The project is being handled through the program Comprehensive Sustainable Systems in Agriculture 2012-2018, which was announced by the Ministry of Agriculture of the Czech Republic. Implementation of the project got under way in 2015, and it will be completed in 2018. This project is being carried out by the Research Institute for Brown Coal, a.s. in collaboration with the Faculty of Environment at the University of J. E. Purkyně in Ústí nad Labem. The theme of the utilization of renewable energy sources is linked to a sub-objective called "Analysis of the Podkrušnohoří Region", which is currently being addressed.

1 Objective of the Research

The project "Sustainable Forms of Management in an Anthropogenically Burdened Region" deals with the specific issue of one of the most anthropogenically burdened regions not only in the Czech Republic but also in Central Europe, which was part of the so-called Black Triangle formed by the regions illustrated in Fig. 1.



Source: [1]

Fig. 1: *The designated Black Triangle area in Central Europe*

The history of the name Black Triangle dates back to the 1970s. This is the area with the most polluted environment in Central Europe. On the Czech side, it was the Ústí nad Labem, Teplice, Most and Chomutov districts that were most affected in terms of environmental pollution. Other districts on the Czech side – Děčín, Česká Lípa, and Liberec – were polluted from emissions that came partly from Germany (the Hagenwerder power station and the Berzdorf Quarry), but mainly from Poland – The Turów Power Station and Quarry, near the town of Bogatynia.

The greatest problem in the entire Black Triangle area was air pollution from sources at thermal power stations, heating plants, open-cast coal mines, and chemical plants. The main air pollution agents were SO_2, NO_x and dust particles. In the 1980s and 1990s, the values of these agents exceeded the public health limits several times over.

The long-term burden on the environment in the previous period was the reason for its deterioration, and some of its components were also reflected in inhabitants' poor health. Project No. QJ1520307, which is currently being carried out, is contributing to management methods in the region that will create conditions for a lasting improvement in the environment and will create conditions for permanently sustainable development.

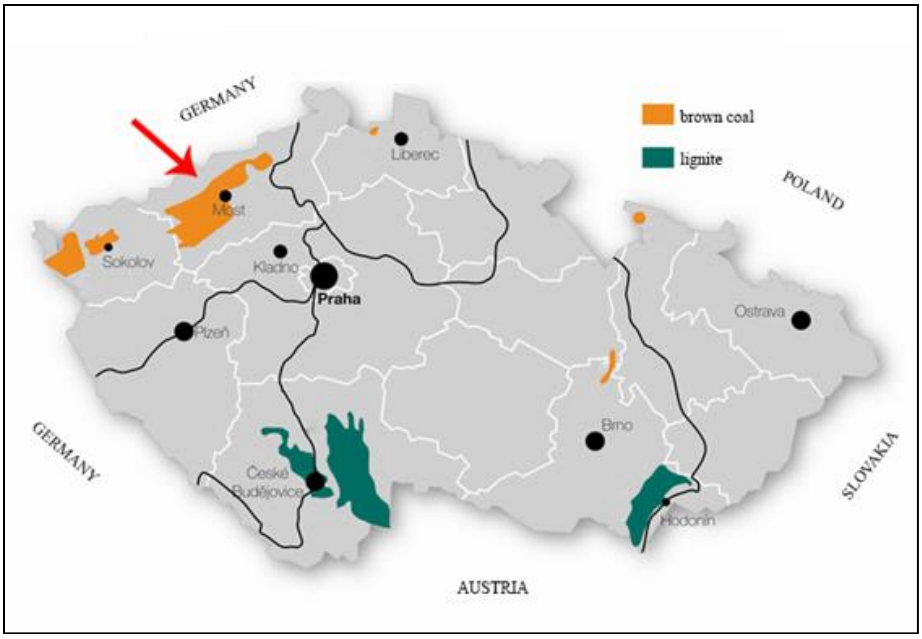
This contribution deals with the project's sub-objectives, which include the presentation of the development of mining activity in the Podkrušnohoří model area and subsequent analysis of the potential use of renewable energy sources in the area of interest.

2 Research Methods

The most anthropogenically burdened region in the Czech Republic is formed by the Chomutov, Most, Teplice and Ústí nad Labem districts (Fig. 2). This region has been significantly affected by intensive mining and industrial activity for almost 200 years. The area is 2,276 km^2 in size and home to 486,000 inhabitants. The area is a typical industrial region, which in the late 1980s was part of the Black Triangle area due to the open-cast mining of brown coal and its combustion in power stations. As a large number of inhabitants live in this region, an attempt is being made to integrate the area into the surrounding landscape in the form of revitalization processes, thereby ensuring the permanently sustainable development of the landscape and society. On October 19th 2015, the Government of the Czech Republic approved new territorial ecological mining limits in the Bílina Quarry via Resolution No. 827, whereby mining limits will be stipulated 500 m from the municipality's built-up area. In the context of this Resolution, the Government of the Czech Republic assessed:

- the economic impacts in terms of the considered variants of the suspension of coal mining limits in the territory of North Bohemia,
- social impacts on individual municipalities and on the Ústí nad Labem region,
- analysis of the need for brown coal supplies for the heating industry,
- quantification of the environmental and health impacts of the open-cast mining of brown coal in the Bílina and Czechoslovak Army quarries,
- use of extracted brown coal in combustion processes for the production of electricity and heat on the territory of the Czech Republic. [2]

With the suspension of mining limits, the anthropogenic burden on the landscape around the Bílina Quarry will also increase. After brown coal mining in the Most Basin has ended, pressure will be placed on the development of alternative energy sources there. Thus, it is essential to analyze the potential of these forms of energy in the model area in order to fulfill the energy consumption requirements of everybody who is currently dependent on its production by the combustion of brown coal.



Source: Own adaptation from [3]

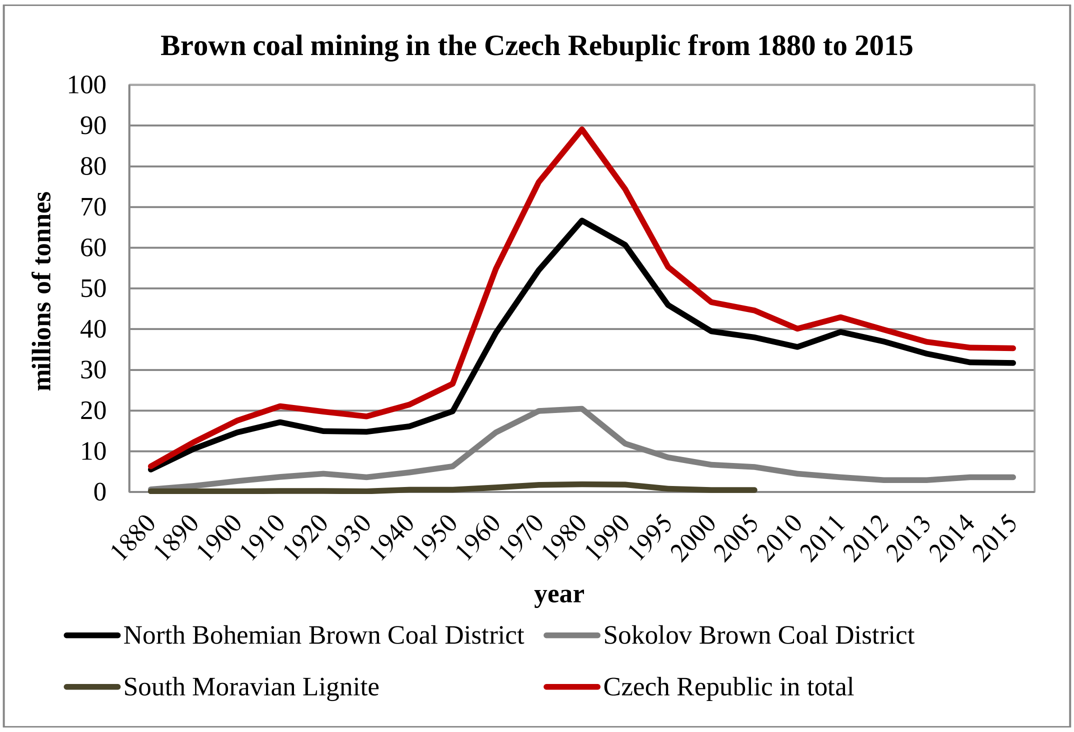
Fig. 2: *Deposits of brown coal and lignite in the Czech Republic*

3 Coal Mining in the Area of Interest

A particularly important source for analyzing the development of coal mining and recultivation in the North Bohemian Brown Coal District was the data from the State Mining Administration (Mining Yearbooks) from 2005-2015. In order to ensure the sustainable development of the landscape after coal mining, it is necessary to follow its revitalization methodology and abide by its individual phases and stages.

Raw material mining is the most serious anthropogenic activity in the region. It includes both underground and open-cast mining. In North Bohemia, the most obvious anthropogenic geomorphology, i.e. the result of man's direct interference with the original land surface, is in the area of open-cast brown coal quarries. Not only the physical-chemical effects, such as dust, noise and fumes have had an impact, but also the aesthetic perception has been – and continues to be – very strong. Of the total expanse of the model area (2,276 km^2), a significant part of its southern, basinal section is directly disrupted by open-cast mining, large-scale external dumps and other related anthropogenic interference with the region and its vegetation. Since the 1960s, 116 municipalities or parts thereof have been liquidated there, including the historical part of the city of Most. At the same time, almost 90,000 people have been relocated. The concentration of production activities leads to enormous emissions and the resulting impact of air pollution on the region's landscape. [4]

The growth in electricity production, the chemical industry and metal processing in the region have been contingent on the supplies of brown coal in the model area, which have been mined industrially since around 1850. From its beginnings until the present day, open-cast brown coal mining has affected an area of approximately 250 km^2, reaching its peak with a volume of almost 70 million t/year in the 1980s (Fig. 3).



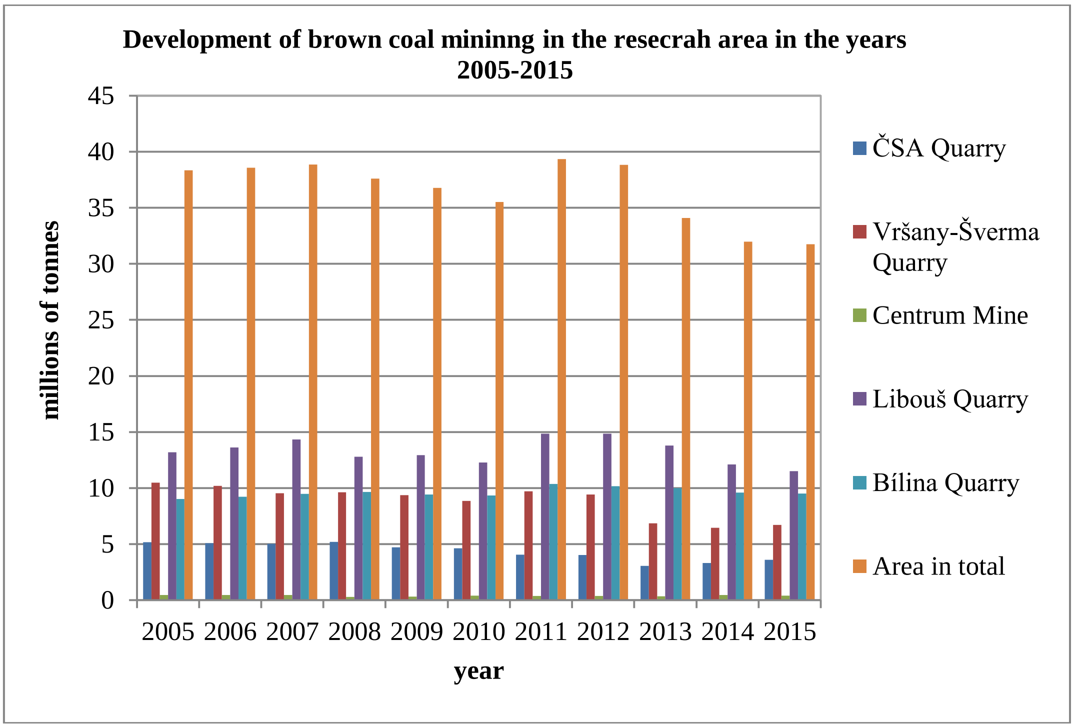
Source: Own adaptation from [5]

Fig. 3: *Historical development of brown coal mining in the Czech Republic since 1880*

In 2015, mining in the Most Basin reached 31.65 million tons, and the production on this territory under the Ore Mountains is carried out by the following quarries:

- Czechoslovak Army Quarry – Severní Energetická a.s.,
- Vršany Quarry – Šverma – Vršanská Uhelná a.s.,
- Libouš Quarry – Severočeské Doly a.s., Nástup Tušimice Quarries,
- Bílina Quarry – Severočeské Doly a.s. Bílina Quarries.

The last underground quarry in the basin, the Centrum (Kohinoor) Quarry, mined its last coal on April 1, 2016, and the quarry is now gradually being closed down. An overview of mining in individual quarries and the Centrum Quarry over the last 10 years is shown in Fig. 4. According to current plans, given a similar annual mining volume and in compliance with the existing limits in the Czechoslovak Army Quarry, mining in the North Bohemian Brown Coal District (SHR) should end between 2050 and 2055 [6] by mining the last of the coal supplies in the Vršany Quarry in the Slatinice extraction area and the Bílina Quarry, whose continuation beyond the originally stipulated limits was decided on by the government in October 2015.



Source: Own adaptation from [5]

Fig. 4: *Development of coal mining in SHR in 2005-2015*

Some 89.7% (31.65 million tons) of brown coal in the Czech Republic was mined in the model area in 2015, and approximately 40% of the installed power generation capacity of the Czech Republic is concentrated there on the basis of solid fossil fuels (steam-electric power stations), for which approximately 85% of the fuel base comprises brown coal. The indicated concentration of production activities leads to enormous emissions and the resulting impact of air pollution on the region's landscape, and it plays a part in the comparatively poor evaluation of the region's environmental quality factor within the scope of the Czech Republic.

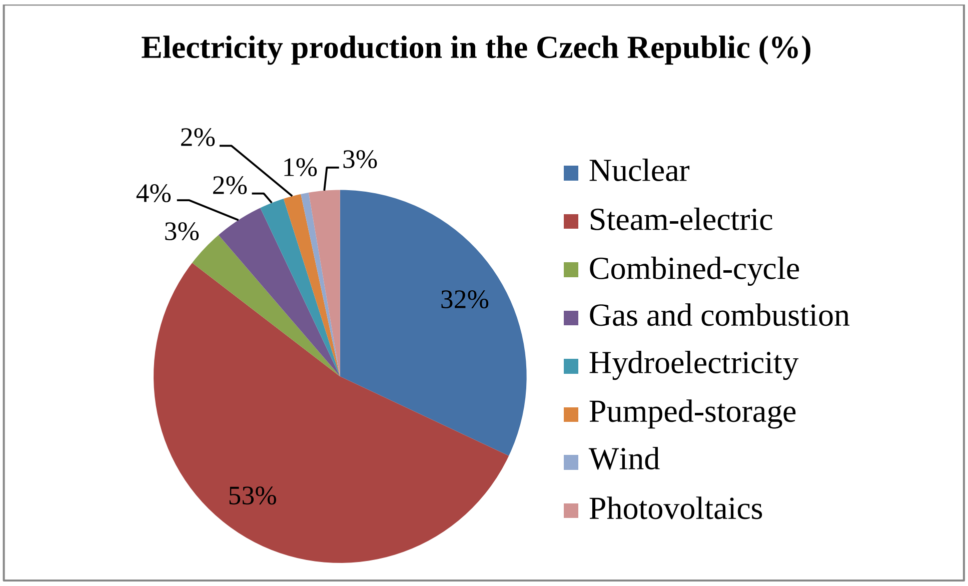
4 Renewable Energy Resources in the Czech Republic

To achieve the objectives of permanently sustainable development in the region, we must take gradual steps to secure the creation and development of legislation and measures in the price area, and limit the use of non-renewable sources. The main measures that will help us achieve these objectives are fuel economy and meeting consumption needs through renewable sources. From the perspective of sustainable development, it would be appropriate to fiscally differentiate between non-renewable and renewable sources; to impose tax penalties on non-renewable sources, particularly carbonaceous fuels, and provide tax breaks for demonstrably economical technology and business. A duty should be imposed on the import of energy-demanding technology, and, on the contrary, economical technology that utilizes renewable sources should be exempt from fees. At the same time, the sale of energy abroad should not be supported.

Energy has great significance for individual branches of the national economy. Any movement in the price area will affect costs in all branches, including the population's expenses. Energy prices also significantly affect the structure of industry, utilization of renewable resources, prices of products etc. [7]

The essence of the problem lies in the fact that, if the current trend continues, all non-renewable sources will be exhausted in a short time, which is why alternative renewable energy sources (RES) must gradually be found to take their place.

Given the level of GDP created, the Czech Republic consumes more primary energy sources (PES) and electricity than the average for EU countries. The relatively higher consumption of PES per unit of GDP in the Czech Republic is because the structure of the industry is different from the EU-15 sectoral structure, whereby domestic energy sources – black and brown coal, uranium and biomass – are utilized on a long-term basis. In 2015, a significant share of the power industry in the Czech Republic was taken up by coal and gas (approximately 60%) as well as uranium, via nuclear energy (approximately 32%). There has been a gross increase in the share of renewable sources in electricity production in the Czech Republic of 2% compared to the previous year (6%) (Fig. 5).



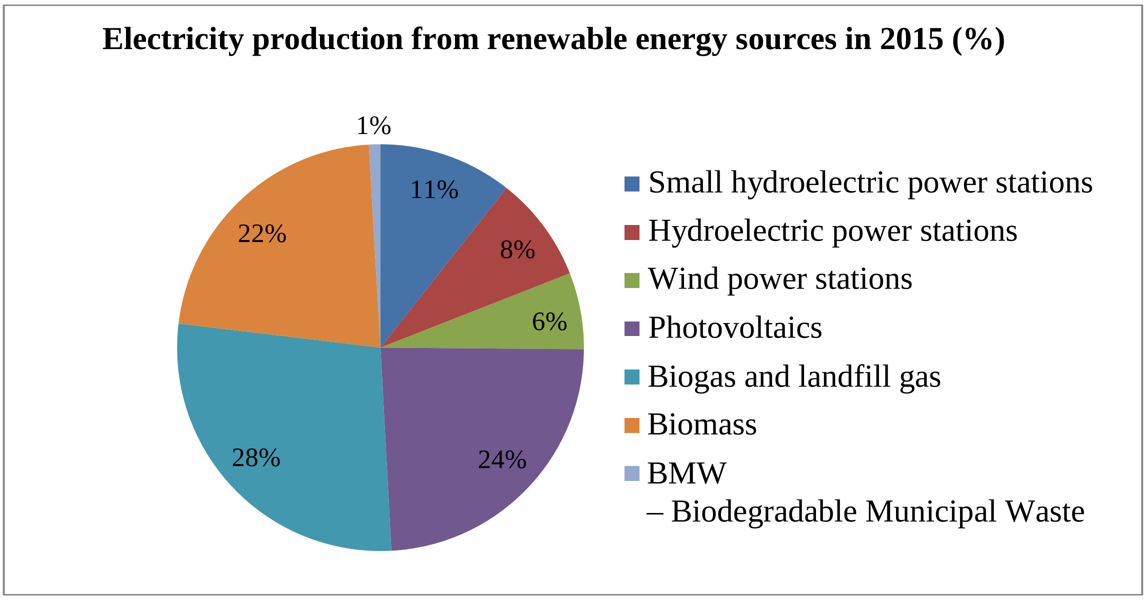
Source: Own adaptation from [8]

Fig. 5: *Gross electricity production in the Czech Republic in 2015*

The share of RES in domestic gross consumption (MWh) was 13.27% in 2015. In comparison with 2014, this means an increase in the share of RES in domestic gross consumption in the Czech Republic of 0.1%.

Overall, landfill gas and biogas still assume the largest share of energy production from renewable sources (28%), and this category has been constantly on the rise since 2006. In 2015, the share of photovoltaic, 24%, was the largest since 2006. The same development applies for biomass, which had a 22% share in the production of electricity from RES in the Czech Republic in 2015. In 2015, wind power stations were also at their greatest year-on-year maximum in the share of electricity production (6%). On the contrary, hydroelectric power stations above 10 MW saw their biggest decline in their share of electricity production since 2006 (8%) (Fig. 6). [8]

At present, in terms of legal regulations, the use of biofuels in the Czech Republic is stipulated mainly by the obligation to mix them with mineral fuels. This obligation was first introduced in September 2007 for the FAME (fatty acid methyl ester) additive to diesel (2% by volume), and since 2008 it has been applied to the addition of bio ethanol to petrol. The domestic production and import of bio ethanol in 2015 remained at almost the same level as in 2014. [9]



Source: Own adaptation from [8]

Fig. 6: *Electricity production from RES in 2015 (%)*

5 Renewable Energy Resources in the Model Area

The Annual Report on the Operation of the Power Industry in the Czech Republic for 2015 shows that energy production in most regions is dominated by steam-electric power stations, mainly in the Ústí nad Labem, Central Bohemian and Moravian-Silesian regions. In the Ústí nad Labem region, a significant proportion of energy production is by combined-cycle power stations, as it is in the Karlovy Vary region. In the South Bohemian region and Vysočina region, the energy production mainly comes from nuclear power stations. In terms of RES, a significant proportion of energy is produced by hydroelectric power stations in the Central Bohemian region; in Vysočina and the Olomouc region, pumped-storage power stations are relatively dominant; and photovoltaic account for a small proportion of energy production in the Central Bohemian, Ústí nad Labem, Plzeň, South Bohemian, Zlín and particularly South Moravian regions.

In order to ensure the sustainable development of the model area after the end of mining and the use of brown coal in the power industry, we have to carry out a detailed analysis of the potential of renewable sources to ensure that society's energy demands are covered. First, however, we have to analyze the existing capacity of all thermal power stations that are found in the Podkrušnohoří region. The ČEZ Group operates coal-fired power stations and heating plants in a total of 13 localities on the territory of the Czech Republic. Most of them burn North Bohemian brown coal and, for practical reasons, they are situated in the immediate vicinity of large quarries in North and Northwest Bohemia. They include the following coal-fired power stations: Ledvice, Počerady I., Počerady II., Prunéřov, Tušimice I. and Tušimice II., which currently have an installed capacity in all power station blocks of 3,620 MW. [10]

For now, the anthropogenically burdened territory of North Bohemia has the highest installed capacity within the scope of RES energy from solar sources (108.21 MW), as set forth in Table 1. In this case, however, this is not an efficient or sustainable choice, as this high installed capacity came about because the construction of a solar power station was economically advantageous while a subsidy program was in place. This was caused by the abnormal and unsuitable construction of solar farms without taking into account the return on investment or the suitability of the installation. At the same time, the Agricultural Land Fund took effect (Fig. 7).

Source: Photo by Vráblík, 2015

Fig. 7: *Photovoltaic power station in Moldava in the Ore Mountains (Teplice district)*

Renewable energy from hydroelectric power stations is also relatively well represented in the model area; nevertheless, it does not seem to have the potential for the future, as there is currently a problem with drought and the water supply, both there and in the Czech Republic in general. The highest installed capacity is on the Elbe River (19.5 MW). Biomass processed in biogas stations has a certain future in this region if it receives more support. At present, 4.2 MW is installed in the area of interest. These stations have an advantage in that they process both animal and plant waste. Energy from wind power stations has the greatest potential for the region; this is a mountainous area, where regular air currents are typical. At present, 87 MW is installed in the Ore Mountains. However, this method has caused a great deal of controversy, as the inhabitants have criticized certain aspects such as noise, unsightliness and the danger to the fauna living in the vicinity.

Tab. 1: *Overview of the installed RES capacity in the analyzed area for 2015*

District	**Installed RES capacity [MW]**			
	Wind	**Hydroelectricity**	**Solar**	**Biogas**
Chomutov	55.80	16.12	47.30	0.99
Most	17.00	7.62	8.68	0.77
Teplice	10.00	0.00	40.82	0.68
Ústí nad Labem	4.00	19.50	11.41	1.76
MA in total	86.80	43.24	108.21	4.20

Source: Own adaptation from [11], [8], [12], [13]

Every region should be approached individually in terms of its geographic and climatic parameters and the population's priorities and requirements. In this regard, the Czech Republic has limited options for utilizing RES because there aren't suitable conditions for most of them here. A comparison of the installed capacity of coal fired power stations in the Podkrušnohoří region (3,620 MW) with a total installed capacity of RES in the analyzed area of 242.4 MW shows the long-term task involved in searching for other suitable localities for RES as future alternatives after the mining of brown coal comes to an end in 2050.

Geothermal energy is now becoming one of the most attractive sources of renewable energy. Approximately 6,000 MW of capacity is installed in geothermal power stations worldwide, which is only a minute fraction of the overall potential. Countries that actively utilize geothermal energy include Iceland, New Zealand, Japan, the United States and others. For example, the geothermal projects realized in Germany – Altheim and Unterhaching (Bavaria) and Landau (Rhineland) – can serve as positive examples of the utilization of this source in Europe. In the Czech Republic, a similar example is the town of Litoměřice (Ústí nad Labem region).

In the research assessment of the geothermal potential, the Czech Republic is not lagging behind other countries in the world. The geothermal potential in the individual parts of our region varies considerably, particularly in relation to geothermal, geological and hydrogeological conditions. When incorporating the territory of a certain region, we must divide it into areas that are most suitable for the utilization of geothermal energy for individual buildings and areas that are suitable for larger sources that can be used for the large-scale supply of heat or electrical energy production. Based on experience from other countries with similar geological structures, the Czech Republic also has potential geothermal energy sources. Heat flow anomalies have been registered in the area of the Ohárecko Rift, i.e. the Podkrušnohoří region, the western part of the Czech chalk table and the Ostravsko-Karvinská Basin. These are so-called low temperature hydrothermal sources, i.e. to a temperature of 100 degrees, and the geothermal energy of so-called hot dry rocks, whose potential at depths of 3,000-5,000 m is considerably higher. Research into, and utilization of, these sources should be supported more in the future. [14]

Various studies show that the gradual growth of renewable sources and the energy-related modernization of buildings in the Ústí nad Labem region can create as much as 2,300 jobs. Significant options for the more efficient handling of thermal energy in the Ústí nad Labem region also include the energy-related renovation of buildings. Quality reconstruction using wall insulation, window replacement and the use of modern managed ventilation technology with heat recuperation will save an amount of heat corresponding to normal consumption by almost 60,000 households and 33,000 family homes [15].

Conclusion

Due to lower fossil fuel supplies, the energy situation will be a serious problem in the third millennium, and it requires a solution. Another topical issue, particularly under the conditions existing in the Czech Republic, will also be the search for, and utilization of, other sources within the scope of RES, for example the cultivation of biomass for energy purposes on the recultivated territory of the Podkrušnohoří dumps, and the use of additional solar sources in brownfield-type areas and buildings.

The issue of the power industry and energy use must be globally linked with current opinions on options for dealing with the climate change. Carbon dioxide emissions will have to be reduced significantly in the coming decades, and adaptive measures will gradually have to be taken to prepare for possible climate change.

Permanently sustainable development is a basic prerequisite for the development of the contemporary society, and should be the top priority during planning processes. In the future, in the anthropogenically burdened region of Podkrušnohoří, we can consider the potential use of not just newly created bodies of water within the scope of hydrological recultivation (Bílina Quarry, Czechoslovak Army Quarry, Vršany Quarry), but also the utilization of the potential of renewable energy sources.

Acknowledgements

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PROBLEMATIKA ENERGETICKÝCH ZDROJŮ V PODKRUŠNOHOŘÍ

Těžba uhlí má prokázané negativní dopady na území a krajinu. S rostoucím počtem obyvatel jsou stále zvyšovány nároky na energetickou spotřebu. Pro budoucnost je důležité se zaměřit především na obnovitelné zdroje energie, které zajistí udržitelný vývoj životního prostředí a společnosti. Tento přípěvek se zabývá oblastí, která má v České republice v tomto směru největší problémy, a to jsou Severní Čechy (okresy Chomutov, Most, Teplice, Ústí nad Labem). Jde o oblast s výraznými antropogenními zásahy zejména kvůli intenzivní těžbě hnědého uhlí a v souvislosti s energetikou. V současné době došlo v oblasti Podkrušnohoří k částečnému prolomení limitů těžby na lomu Bílina, a proto bude do budoucna velice důležitá obnova území v rámci rekultivací a revitalizací. Zároveň příspěvek obsahuje možné směřování v oblasti energetiky, tedy jaké obnovitelné zdroje energie v Podkrušnohoří mají potenciální využití po ukončení těžby na jednotlivých lomech po roce 2050.

PROBLEME DER ENERGIEN IM VORERZGEBIRGE

Kohleförderung hat nachweisbar negative Auswirkungen auf die Umgebung und die Landschaft. Mit steigender Einwohnerzahl werden die Ansprüche an den Energieverbrauch ständig erhöht. Es ist wichtig, sich für die Zukunft vor allem auf erneuerbare Energien zu konzentrieren, die die nachhaltige Entwicklung der Umwelt und der Gesellschaft sichern. Dieser Beitrag beschäftigt sich mit dem Gebiet, das in der Tschechischen Republik in dieser Hinsicht die größten Probleme hat, und zwar Nordböhmen (die Landkreise Chomutov, Most, Teplice, Ústí nad Labem). Es geht um ein Gebiet mit markanten anthropogenen Eingriffen besonders wegen der intensiven Förderung von Braunkohle und im Zusammenhang mit der Energiewirtschaft. Gegenwärtig ist es im Gebiet des Vorerzgebirges zur teilweisen Durchbrechung der Förderlimits im Bruch Bílina gekommen, und deshalb werden die Erneuerung des Gebiets im Rahmen der Rekultivierung und Revitalisierung sehr wichtig sein. Gleichzeitig enthält der Beitrag eine mögliche Orientierung auf dem Gebiet der Energiewirtschaft, also welche erneuerbaren Energien im Vorerzgebirge nach Beendigung der Förderung in den einzelnen Brüchen nach 2050 eine mögliche Verwendung finden werden.

ZASOBY ENERGETYCZNE NA PODGÓRZU RUDAWSKIM

Wydobycie węgla wpływa zdecydowanie negatywnie na obszar i krajobraz. Wraz ze wzrostem liczby mieszkańców nieustannie zwiększa się zapotrzebowanie na energię. Na przyszłość ważne jest skoncentrowanie się przede wszystkim na odnawialnych źródłach energii, które zapewnią zrównoważony rozwój środowiska naturalnego i społeczeństwa. Niniejszy artykuł dotyczy obszaru, który pod tym względem boryka się z największymi w skali kraju problemami, tj. Północnych Czech (powiatów Chomutov, Most, Teplice, Ústí nad Labem). Jest to region o znacznych zmianach antropogenicznych, związanych przede wszystkim z intensywnym wydobyciem węgla brunatnego oraz z energetyką. Aktualnie w regionie Podgórza Rudawskiego przekroczono częściowo limity wydobycia w kopalni odkrywkowej Bílina, w związku z czym w przyszłości bardzo ważne będzie zrewitalizowanie i zrekultywowanie tych terenów. Artykuł przedstawia także możliwe kierunki w dziedzinie rozwoju energetyki pokazując, z jakich odnawialnych źródeł energii będzie można potencjalnie korzystać na Podgórzu Rudawskim po zakończeniu wydobycia w poszczególnych kopalniach po 2050 roku.

Miscellanea

CHITIN-BASED BIOMONITORING: USE LIVING ARTHROPODS OR CARRY SAMPLERS BY ROVS?

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Abstract

Chitin which is located at outer surface of arthropods and some other organisms adsorbs quite a variety of possible environmental pollutants such as heavy-metal ions and –complexes and biomethylation products; thus biomonitoring is feasible without passing (and thus probably fractionating) analytes through metabolism. Isolated (from crab peeling) and grafted, chitin likewise acts as a sorbent, even in conditions which a living animal would not endure. Techniques originally developed in the author´s lab to maintain animal integrity throughout sampling protocols are now used for analytical workup omitting sample digestion. Hazardous or poorly accessible sites may be investigated using ROVs which deploy chitin samples to the site for the 10 min until adsorption is usually completed.

Keywords

Chitin; Environmental sampling by adsorption; Biopolymer solutions; Analytical workup omitting sample digestion; Addressing hazardous sites by purposely designed ROVs.

Introduction

The previously established, e.g., [12], [13], [14], [15], use of native arthropod chitin (rather than [hydrolyzed] chitosan) to withhold/extract “heavy metal” pollutants or neutral or cationic organics ([1], [3], [11]) from waste water or from solutions obtained by dissolving processed nuclear fuel rods etc. (containing ^{106}Ru-NO complexes, ^{90}Sr, radionuclides of Ba, La, Ce, etc., [13]) was developed by the author and his team into a method of estimating element concentrations by a simple contact with different media/matrices, e.g., [7]. This does encompass rather diverse speciation forms; chemical activities of the analytes are measured rather than total concentrations. This also holds for chemically connected different phases (e.g. inundated sediment, water above).

An obvious application in environmental monitoring to be based on living arthropods was finally developed – which was in fact demonstrated in our (IHI Zittau) lab – to obtain this kind of information without harming or killing the animals[1] [2]. This does permit the use of protected or rare arthropod species (which holds for most which are sufficiently large, except of millipedes). However, the range/severity of environmental pollution living arthropods of sufficient size can both endure; and thus sample by either outer (i.e., chitin) covers or internal organs (muscles, fat, hemolymph (cp. [9]) is limited. Hence we switched to using isolated

[1] Whereas chitin also is produced by fungi, some bacteria and even certain vertebrates (blenniid fishes, forming their fin fortifications, [17]), the focus here is on arthropods (insects, spiders, isopods, millipedes etc.) as only in these organisms – not in fungi (which are no animals at all) nor in fishes or bacteria – chitin actually forms interfaces directly exposed to the environment

chitin grafted on glass slides and we are currently developing devices for location of samples without humans being directly involved in sampling, thus enabling safe studies of hazardous imminent disaster sites, active volcanoes and their vents or in the deep ocean.

1 Materials and Methods

- Living field crickets (*Gryllus assimilis*) (obtained from a local pet shop, intended as food for reptiles, spiders, large fishes, etc.),
- Chitin flakes from peeled marine crab *Pandalus borealis* (Sigma-Aldrich), checked for background levels of many metals in our lab by digestion, ICP-MS,
- Metal-free glue to be photohardened by violet or UV light to attach chitin to glass slides or other supports (Solacor™),
- Dimethyl formamide 99.8%, water-free, certified for trace metal contents (Sigma-Aldrich),
- Lithium perchlorate anhydrous, "battery-grade", certified for trace metal contents (Sigma-Aldrich),
- Strongly acidic cation exchanger Amberlite H-120, either employed in its native state or pre-treated by
- tris-n-butyl amine (both Sigma-Aldrich),
- dilute (1%) nitric acid (Merck Suprapur™, diluted with deionized water),
- several salts and minerals representing more or less insoluble forms of chemical elements such as Be, Al, Pb, Mn, Fe, Co, Cu, Zn, Cd, Pb, REEs, like beryl, *Schalenblende* (a layered Zn/Cd- and Fe/Pb sulfide from Poland), chalcopyrite, La2O3, LaCoSr ferrite, mixed (Ce, REE´) oxides or anhydrous CoCl2 (diverse mineral vendors, Sigma-Aldrich),
- microscope glass slides,
- nylon™ mesh bags for keeping mixed sample arrays (Fig.1) or retaining the ion exchanger resin.

Besides the data reported by vendors, all the items were analyzed for metal contents in this lab too.

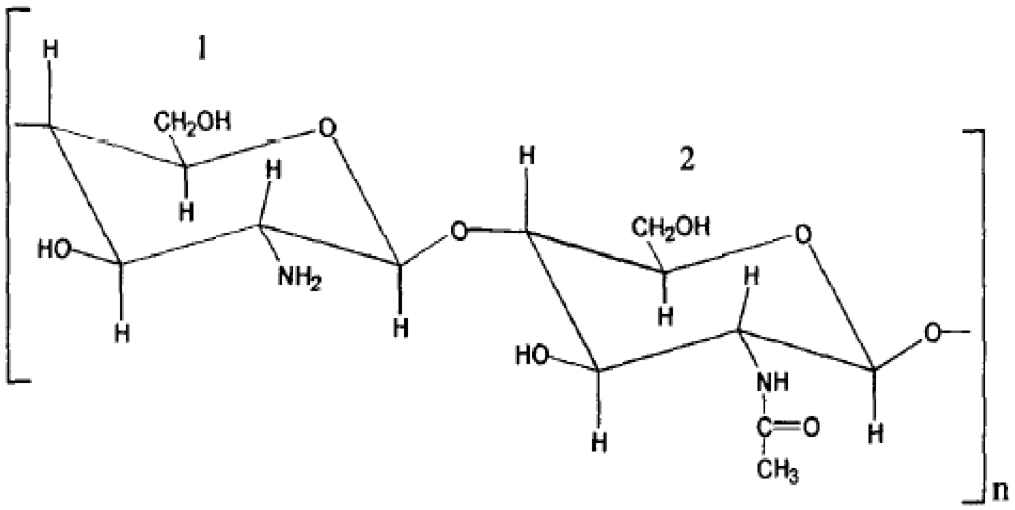
Source: Photo courtesy of G. Kosior, Poland 2015

Fig. 1: *A mesh bag containing dried (thermally devitalized) aquatic moss (right, green) and a glass slide partly covered by chitin (left) for comparative studies of metal retention. Whereas lab experiments showed that adsorption was essentially completed to equilibrium within 10 min except for very high levels of humic acids, these assemblies were exposed to water (a mountain creek in Poland) for periods up to 15 days, assuring constancy of metal levels measured except for two cases of ongoing photochemical deposition (U, Ag) and surface decomposition upon the longest expositions.*

2 Properties of Chitin

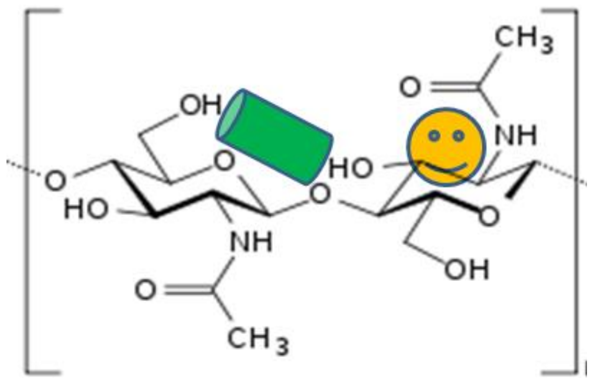
Chitin retains a couple of quite different chemical species to which it is exposed from either gas-, aq., organic solvent- or solid phases ([13], [14], [1], [2], [3], Schieritz & Fränzle 2014, unpublished work). Experiments on vertical migration of adsorbed metals into the deeper chitin layers showed [8] that in some divalent cations (Cu, Ni, Pb) substantial parts of total analyte inventory are retained in the uppermost, probably air-oxidized 2 µm-layer of chitin, with only the remainder passing on to form a more or less distinctive diffusion front whereas most make their way to deeper layers of chitin completely. Primary investigations on crab chitin from Pandalus borealis showed that except for Al, Fe and Ti background levels[2] of chitin used were very low, owing to the minute solubilities of most "heavy metals" other than Mo, Cr in conditions of oxygenated sea water (pH = 8.2). This improves the possible sensitivity of detection of the very analytes in environmental samples.

[2] Levels of As detected in such environmental samples from quite diverse sites in Mongolia suggest a fairly highly As pollution (Fränzle et al., to be published); whereas quaternary arsonium salts such as arsenobetaine or tertiary arsine oxides are quite typical in marine crustaceans [10], the actual As background in the employed chitin is very low.



Source: [16]

Fig. 2: *Structure of chitin*



Source: [7]

Fig. 3: *Probable binding sites and –modes of metal cations (orange sphere) and H-bonding anions (green cylinder, meant to symbolize e.g. cyanide). Complexation to carboxamides mainly operates via O rather than amide N.*

Adsorption of organometal compounds like $Pn(CH_3)_3$ (Pn = Sb or Bi) or homoleptic metal carbonyls (M = fe, Mo, or W) which both occur in landfill and sewage gases ([5], [6]) was investigated, including additions of oxidants like iodine or O_2/Co(II)amino acid complex-combinations (which modify [likely enhance] binding properties by formation of oxospecies or of $[M(CO)_nI_x]^+$ or Me_3PnI^+ ions, to understand the effects of oxygenation by soilborne exoperoxygenases produced by fungi and bacteria. However, corresponding effects were not observed unless for unrealistically high substrate levels (Schieritz & Fränzle 2014, unpublished work). Preliminary data indicate that with $[Mo(CO)_6]$ saturation is reached at about the level detected in landfill gases (≈ 1ppbv, see [5]). Substantial parts of it can be thermally desorbed in a headspace system and retrieved/identified in a GC/MS setup.

3 Obtaining Samples by Grafted Chitin and Processing Them

The procedure of sampling was described elsewhere; thus we may restrict to some brief outline here:

After exposition of the chitin surface (bright spot in left part of Fig. 1) to water, air or wet sediment, a concentrated solution (1.6 M/kg) of $LiClO_4$ in DMF is pipetted on the chitin surface (about 0.1 ml/cm^2 of chitin), dissolving the uppermost layer in DMF/Li^+ medium, but not possible metal-containing particles[3] adhering to the surface. For multiple ablations, this procedure is repeated up to eight times providing almost planar dissolution of layers some 2 µm thick in each case [8] to pinpoint how deep certain metals have migrated by diffusion. But it is likewise feasible to take eight times this amount and remove some 15 µm of chitin at once (T. Gebauer 2016, oral communication). Then the solution – still adhering to chitin – is exposed to a small bag containing a cation exchanger resin (300 mg) for 45 s to absorb the metal ions from the metalated chitin solution. Either the polymeric arenesulfonate resin is applied in its native protonated form or after treatment by tributyl amine in CH_3OH, the tributylammonium form can be used. After fixation to ion exchanger, the bag is immersed into 1% nitric acid pumped through it by a syringe several times to unload the ion exchanger. Additionally, this procedure will release metal ions still adhering to chitin as binding to the polymer stops at pH << 3.

4 Results

Large sets of data already or to be published elsewhere ([8], Fränzle, Kosior et al. 2017) show that very different analytical items can be transferred/retrieved from different kinds of fluid or solid matrices by contact of moist solid or aq. slurry/suspension. Respective solid matrices include wood and minerals. Some 10 min-periods of mechanical contact with solids (cardpaper previously exposed to metal-containing components of dyes, fortifying additives [clays delivering Al], wood) suffice to produce a clear and lasting chemical signature in chitin surfaces ([2], [8]) which additionally permits to reconstruct the history of previous exposition of test animals (crickets, wood-wasps or beetles developing or living in wood) during rearing to a considerable number of elements, often including different speciation forms.

The approximate date when this (last) exposition took place can be reconstructed by following the slow vertical diffusion from the interacting surface to deeper layers. These can be dissolved one by one (each some 2 µm) removing almost plane layers and then analyzed in order to determine the extent of migration which, of course, increases with time while for M = Ni, Cu or Pb a substantial part of total sorbate remains next to the surface even months after exposition, with only the remaining 30 – 55% migrating into "bulk" chitin. In lower layers, several elements, most pronounced Co (Co^{2+}), Mn and Pb, produce diffusion fronts as clear maxima after several months of sample storage while levels of elements forming oxoanions like As, Mo tend to steadily decrease when changing into deeper layers. This also holds for organometals present in landfill vent gases (or others, such as volatile [e.g. Fe(III), Al, Sb] chlorides and metal carbonyls, in volcano/fumarole vents); recovery rates were studied in two different setups. Except for REEs, recovery rates measured using perchlorates, chlorides or para-toluene sulfonates of the respective elements added as DMF solutions to a previously non-metalized chitin solution in DMF/$LiClO_4$ will be higher and scatter (RSD) in data much smaller when using the Bu_3NH-modified resin.

Thus, this latter method is selected for actual environmental monitoring even though retrieval is smaller than with the original H^+ form for REEs ([4], [8], Fränzle et al. 2016); among the various REEs so far studied in lab experiments which revealed competition and fractionation from mixed oxides in favor of heavier, smaller-ion REEs (Sm, Gd vs. La, Ce) only Ce, for its

[3] As a rule, metal salts other than perchlorates, chlorides, acetates or trifluoromethanesulfonates will not dissolve in DMF, hence mineral dusts adhering to chitin flakes are not attacked. This improves resistance towards contamination of the sample during (concerning sediment samples) or after (air or water samples during retrieval and transport) sampling. Nevertheless, we plan to switch to processing the samples to this spot (transfer to ion exchanger or nitric acid) right at the place to exclude a) posterior contamination and b) vertical diffusion of certain (most) analytes within the chitin layers. The latter process would compromise sampling when only a single thin surface layer is removed.

being reasonably abundant in common soil samples, has been studied in our environmental samples so far. In DMF/Li+ solutions of chitin citrate can cleave complexation of Ce (but not trivalent Sm, Eu, or Yb) to chitin, agreeing with studies of ligands effects observed in chitin-based extraction of mixed REE-, LaSrCoFe- and Ni/REE oxides with ligand-free4 and loaded aq. chitin suspensions. Back-exchange using dilute aqueous acid will recover the metal ions and render them in a form useful for ICP-MS- or ICP-OES analysis.

4.1 Sorption and Photosorption

By and large, sorption equilibrium is reached within 10 min, except if there are high levels of humic acids, whereas other ligands to be found in soil liquids or forest waters do not influence either the maximum amount to be bound or the kinetics. Upon prolonged exposition, uranium (probably UO_2^{2+}) and Ag^+ are adsorbed much beyond primary equilibrium, given that there is light shining on the chitin samples. This indicates photochemical deposition of either element, Ag probably as metal nanoparticles, uranium as UO_2. Binding capacities of ground chitin are some 35 – 40 μM/g DM for most di- and trivalent ions.

4.2 Animal-Friendly Ways of Sampling: Implications for Selection of Possible Test Animals

Source: Photo courtesy of A. Bauer 2013

Fig. 4: *Time-zero check of a field cricket (Gryllus assimilis) by the method described in text*

[4] The ligands selected (glycinate, citrate, hydroxamates, humic acids) and their concentrations were meant to simulate soil solutions under different kinds of vegetation.

Source: Photo courtesy of S. Fränzle 2013

Fig. 5: *Field cricket in a microterrarium dwelling on moist silica doped with metal salts or ground minerals at levels of several 100 µg/g. The red color is due to photographic flash.*

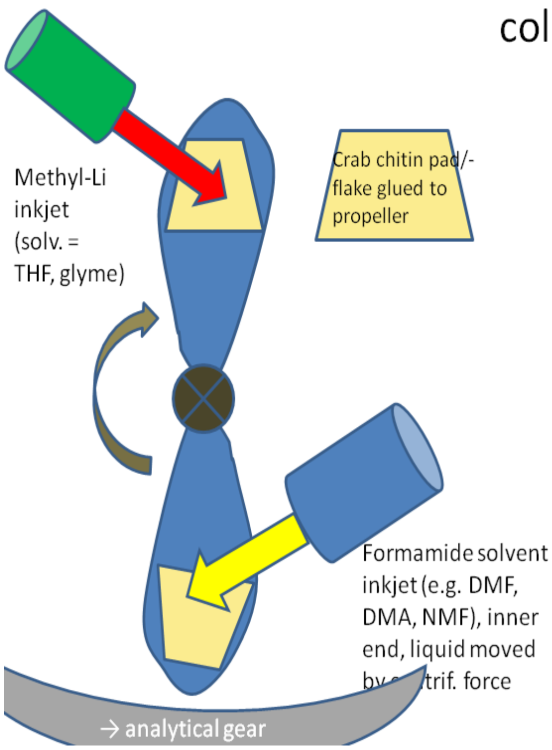
Just a thin layer of chitin is dissolved from the carapace **without harming the animal**[5] which is reversibly immobilized by cooling to $T \approx 0°C$. With the crickets, many specimens were observed moving with their lower abdomina in permanent contact with the model sediment consisting of silica powder for chromatographic purposes and ground minerals or insoluble salts added to it in concentrations selected to represent “Dutch List” intervention levels; these amounts could be readily identified. Although different crickets were observed to differ considerably in self-cleaning activities, the results would be highly reproducible.

5 Discussion

Living arthropods are versatile in chitin-based biomonitoring and can inhabit very diverse habitats and biocoenoses where neither plants (including mosses) nor vertebrates would persist for long or even reproduce. Yet, unless for very specific sites offering the only affluent nutrient sources around, like “black smokers” in the deep ocean, they are unlikely to keep

[5] At least if you (can) avoid getting the solvent into tracheae

close to sites where there is some high load in analytes/pollutants; moreover, they might either flee from or succumb to (even if kept in cages, terrariums or tanks for limited, well-defined periods of time) high levels of pollutants. Accordingly, the most critical sites cannot be measured despite the fact that chitin is a most versatile sorbent. Hence, the author has changed his original attitude, shaped by biomonitoring concepts, towards using chitin samples attached to inorganic supports which can be freely placed almost regardless of local conditions far beyond those required for arthropod survival. Due to low background levels submarine freshwater springs (typically rich in Fe), "black smoker" sites could be detected and investigated in the same manner. By comparison among chitin attached to the outer surface of submersibles, an improved understanding of chemical transport supporting the local biocoenosis can be achieved, like in terrestrial and bog environments, then e.g. using airborne sampling devices (shown in Fig. 6 and 7).



Source: Own

Fig. 6: *Chitin sampling of components of fluids and a method for direct removal to sampling device. The grey curve (bottom) may represent a cation exchanger resin. After binding to the resin, back-elution is affected by 1%-nitric acid and the sample is directly taken to ICP-MS.*

6 ROV Technologies to Dislocate Chitin for Sampling (Status and Outlook)

Accepting grafted chitin to be superior in applicability and reproducibility of results to living, freely swimming or flying or crawling animals means one must design vehicles to get the sampling sheets to the area/sites to be investigated, usually ROVs for reasons soon to be described. The sampling device must remain at the spot just until equilibrium is reached (≈ 10 min), then withdrawing the sampler carrier and returning to the starting site or (more conveniently) moving to another sampling site within one mission. At the present state of technical development, remote control still must be considered superior to operating some fully autonomous systems, whether being airborne, moving on solid ground or water or being a submersible. Possible designs are shown here, one meant for sampling metal contents of leaf litter, topsoil, other soft sediments (penetrating into an anoxic submerged layer in a controlled fashion) and (shallow) water, while the other (fixed to some propeller) should bind analytes from air or water directly.

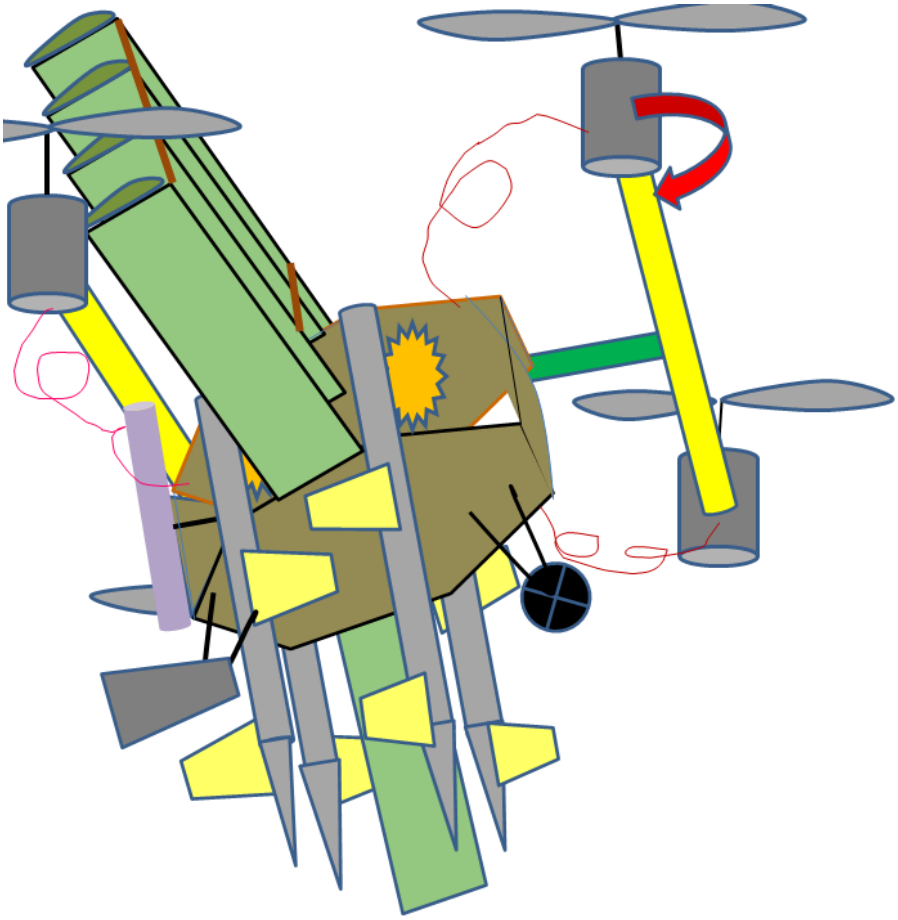


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Fig. 7: *A multicopter drone equipped with stacked wings for more efficient (slow) horizontal flight in between sampling sites. Chitin flakes are fixed to (covers of) retractable poles to be inserted into water or/and soft sediment one by one. Moving front wheels and aft ski towards each other assists re-take-off of plane. The device is kept at one sampling site for some 10 min until equilibrium of chitin adsorption is reached.*

Conclusion

Chitin is a very useful and affordable[6] sorbent material for purposes of environmental analysis. Comparative studies in rivers/creeks, their underlying sediments and mining sites in Mongolia showed, in full accord with the expectations and the fact that chitin does bind the metal ions by complexation and thus does probe their respective chemical potentials, that adsorption from water samples (pH = 5.5 – 7.6) and underneath sediment give almost identical values in still or slowly running waters, with the highest Al readings over/in a clayey river bed (lower Tuul R.) and Cu maxima in runoff waters of a copper mine near Erdenet.

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Dr. Stefan Fränzle

BIOMONITORING NA ZÁKLADĚ CHITINU: POUŽÍT ŽIVÉ ČLENOVCE NEBO ZKOUMAT VZORKY POMOCÍ ROV?

Chitin, který se nachází na vnějším povrchu členovců a některých dalších organismů, absorbuje poměrně širokou škálu látek znečišťujících životní prostředí, jako jsou těžké kovy, komplexní sloučeniny iontů a produkty biometylace. Biomonitoring je tudíž proveditelný, aniž by procházel (a tedy pravděpodobně frakcionoval) analyty prostřednictvím metabolismu. Izolovaný (odlupováním korýšů) a roubovaný chitin rovněž působí jako sorbent, a to i v podmínkách, ve kterých by živá zvířata nepřežila. Techniky, které byly původně vyvinuté v autorově laboratoři s cílem zachovat integritu zvířat v rámci dodržování protokolů pro odběr vzorků, jsou nyní používány pro analytické zpracování, aniž by vzorky byly louhovány. Nebezpečná nebo špatně přístupná místa mohou být zkoumány pomocí ROV. Vzorky chitinu je tak možno zanechat na místě, dokud – po zhruba 10 minutách – nedojde k ukončení absorpce.

AUF CHITIN BASIERENDES BIOMONITORING – VERWENDUNG LEBENDER GLIEDERFÜßER ODER DIE ERFORSCHUNG DER PROBEN MIT HILFE VON ROV?

Chitin, das die äußere Oberfläche von Arthropoden sowie mancher anderer Organismen bildet, adsorbiert eine Vielfalt potenzieller Umweltschadstoffe, darunter Schwermetall-Ionen und –komplexe sowie Biomethylierungsprodukte, was Biomonitoring ohne vorausgehende Fraktionierung im Stoffwechsel ermöglicht. Isoliertes (aus marinen Krabben) und trägerfixiertes Chitin fungiert als Sorbens auch unter Bedingungen, die ein lebendes Tier nicht überstünde. Die Methoden, die im Labor des Autors entwickelt wurden zu dem Zweck, Versuchstiere auch bei mehrfacher Beprobung am Leben zu erhalten, dienen jetzt zur analytischen Bearbeitung. Schwer oder nur unter Gefahren zugängliche Standorte sollen künftig mit ROVs („Drohnen“, „Rover“), die an den Auslegern Chitinproben tragen, untersucht werden, wobei 10 Minuten am Messstandort für die Adsorption ausreichen.

BIOMONITORING NA PODSTAWIE CHITYNY: ZASTOSOWANIE ŻYWYCH STAWONOGÓW LUB BADANIE PRÓBEK PRZ POMOCY ROV?

Chityna, znajdująca się w zewnętrznej warstwie stawonogów i niektórych innych organizmów, pochłania stosunkowo dużą ilość substancji zanieczyszczających środowisko, takich jak metale ciężkie, kompleksowe związki jonów i produkty biometylacji. Biomonitoring może być więc przeprowadzony bez konieczności wykorzystania (czyli prawdopodobnie frakcjonowania) analitów w procesie metabolizmu. Także odizolowana (zdjęta ze skorupiaków) chityna działa jako pochłaniacz, zachowując te cechy także w warunkach, w których żywe organizmy by nie przetrwały. Techniki, które opracowano początkowo w laboratorium autora w celu zachowania integralności zwierząt w ramach przestrzegania protokołów pobrania próbek, stosowane są obecnie do obróbki analitycznej bez potrzeby namaczania próbek. Miejsca niebezpieczne lub trudno dostępne można badać przy pomocy ROV. Próbki chityny można dzięki temu pozostawić na miejscu, dopóki – po około 10 minutach – proces absorpcji się nie zakończy.

Developing and Implementing Two-Step Adams-Bashforth-Moulton Method with Variable Stepsize for the Simulation Tool DynStar

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Abstract

The simulation tool DynStar, created by Hochschule Zittau/Görlitz IPM department, was previously using only single-step methods to solve differential equations. This paper describes the development of a multiple step method to complement the others. The Introduction gives the reader a better idea why a multiple step method can be useful. The theory part is focused on the two-step Adams-Bashforth-Moulton method and how it is possible to make the formulas suitable for variable stepsize. Further, an algorithm is developed to solve the differential equations, using the ABM formulas and adjusting the stepsize according to the error between the prediction and the correction. This is described in the Implementation section. Finally, the performance of the ABM method is compared with RK4 and the Hanna method in the Results section.

Keywords

Adams-Bashforth-Moulton; Multistep method; Variable stepsize; Numerical solution; Ordinary differential equation; Initial-value problem; Hanna method.

Introduction

In engineering, it is often necessary to simulate the behaviour of real-life systems. For this, a mathematical model that describes the system is needed. When taking into account the speed of some variations, the description may contain derivatives. This means that you will end up with one or more differential equations in the model. Then you are left with the problem of solving these equations, which can be done analytically or numerically. In the era of computers, numerical solving techniques have become increasingly important.

Considering an initial-value problem $y' = f(x, y)$ and $y(x_0) = y_0$, many methods have been studied to solve this differential equation numerically [1]. The simplest one is undoubtedly the (forward) Euler method, where the following value y_{n+1} is calculated as:

$$y_{n+1} = y_n + h \cdot f(x_n, y_n) \tag{1}$$

Of course, such a formula cannot be used in practice because it generally will not give an accurate result. An attempt to construct a more reliable method has led to the improved Euler method, which uses the average of the slopes in (x_n, y_n) and (x_{n+1}, y_{n+1}). Hence y_{n+1} is calculated implicitly:

$$y_{n+1} = y_n + \frac{h}{2}\left(f(x_n, y_n) + f(x_{n+1}, y_{n+1})\right) \tag{2}$$

Solving an implicit equation on its own can be difficult because it leads to a non-linear problem. However, this difficulty can be avoided by combining the implicit formula with an explicit one in a predictor-corrector scheme; in this case the forward Euler method would be the ideal choice. Unfortunately, the accuracy of the improved Euler method is still disappointing.

Finally, generalization of the Euler formulas was created, which is now known as the Runge-Kutta method. It uses a weighted average of slopes in the interval $x_n \leq x \leq x_{n+1}$.

$$y_{n+1} = y_n + h(w_1 k_1 + w_2 k_2 + \cdots + w_m k_m) \tag{3}$$

It can be concluded that the Euler method and the improved Euler method are in fact Runge-Kutta methods of the first and second order respectively. The formulas that are most commonly used, because they are very accurate and still easy to implement, are of the fourth order.

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{4}$$

$$\begin{aligned} k_1 &= f(x_n, y_n) \\ k_2 &= f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}h \cdot k_1) \\ k_3 &= f(x_n + \frac{1}{2}h, y_n + \frac{1}{2}h \cdot k_2) \\ k_4 &= f(x_n + h, y_n + h \cdot k_3) \end{aligned}$$

Even though RK4 is popular for its accuracy, it has the major disadvantage that in each step the function must be calculated four times. When function evaluations are expensive, this can seriously prolong the runtime. A solution is found in the category of multistep methods. Notice that the methods mentioned above are all single-step methods because in order to compute the successive value y_{n+1}, information about only one prior value y_n is needed. Multistep methods use several points in the calculation, but they gain efficiency by storing the previous information such that only one new function evaluation has to be computed at each step. To improve the accuracy and stability of the algorithm, one can choose to add a corrector step which also requires an additional function evaluation. This doubles the cost, but it is still an improvement over the Runge-Kutta method. The best-known multistep method is the Adams-Bashforth-Moulton one, which will be discussed in the next section.

1 Theory

Adams-Bashforth and Adams-Moulton are linear multistep methods. This means that the next value y_{n+1} is calculated as a linear combination of various y_i and $f(x_i, y_i)$ from the previous s steps:

$$\begin{aligned} y_{n+1} + a_1 y_n + a_2 y_{n-1} + \cdots + a_s y_{n-s+1} \\ = h\big(b_0 f(x_{n+1}, y_{n+1}) + b_1 f(x_n, y_n) + \cdots + b_s f(x_{n-s+1}, y_{n-s+1})\big) \end{aligned}$$

For Adams-Bashforth, coefficient $a_1 = -1$ and all others $a_2 = \cdots = a_s = 0$. The coefficients b_i are derived by considering the following form:

$$y(x_{n+1}) = y(x_n) + \int_{x_n}^{x_{n+1}} f\big(t, y(t)\big) \cdot dt \approx y(x_n) + \int_{x_n}^{x_{n+1}} p(t) \cdot dt \tag{5}$$

It's possible to replace the function $f(t, y(t))$ by the interpolation polynomial $p(t)$ through the s previous points [2]. After the polynomial is calculated, an expression for the coefficients b_i can be found. For example, the two step Adams-Bashforth formula becomes:

$$y_{n+1} = y_n + h \cdot (\frac{3}{2} f_n - \frac{1}{2} f_{n-1}) \tag{6}$$

However, the integration polynomial was integrated from x_n to x_{n+1}, while its interpolation interval is limited to $[x_{n-s+1}, x_n]$. In general, integration polynomials cannot be used as a reliable approximation outside their interpolation interval. So it is logical to include the point (x_{n+1}, y_{n+1}) in the polynomial and do the calculations again. This results in the implicit Adams-Moulton formulas. Again the two-step formula is shown:

$$y_{n+1} = y_n + h \cdot (\frac{5}{12} f_{n+1} + \frac{8}{12} f_n - \frac{1}{12} f_{n-1}) \tag{7}$$

Adams-Moulton has some great advantages over the explicit Adams-Bashforth [3]. As already mentioned, Adams-Moulton methods give more accurate approximations due to the wider interpolation interval. They also obtain a higher order with the same amount of previous steps and generally, implicit methods are more stable than their explicit counterparts. Of course, the drawback lies in its implicit nature, which makes it difficult to solve as it translates to a non-linear equation.

The way to profit from both methods is to combine them in a predictor-corrector scheme. The explicit Adams-Bashforth method computes a prediction ${y^*}_{n+1}$. At this point, the function evaluation ${f^*}_{n+1}$ is calculated. Then the corrected value y_{n+1} is obtained with the Adams-Moulton method and again, the function is evaluated to use in later steps. This is known as the PECE procedure, but it is also possible to repeat the correction step, for example PECECE or even more. Each additional correction step C makes the result more accurate, but also introduces a new function evaluation E, which partly or completely reverses the advantage that ABM has over RK4. A compromise is made by performing the correction step only once while still ensuring a sufficient accuracy. This is established by starting the calculation over with a smaller stepsize when the correction differs too much from the prediction.

This includes that we are now facing a variable stepsize problem and that formulas (6) and (7) must be adapted, because they assume a constant stepsize. The coefficients b_i depend on the ratio of the stepsizes. That's why they are constant for a fixed stepsize, but at each step they need to be calculated in a variable stepsize problem. There are different ways to make the Adams methods suitable for variable stepsizes, but we will follow a procedure developed by Krogh and described by Lopez and Romay in their paper [4].

The expression of the variable stepsize *k*-step Adams-Bashfort predictor and Adams-Moulton corrector is as follows:

$$p_{n+1} = y_n + h_n \sum_{j=0}^{k-1} g_j(n)\, \beta_j(n)\, \phi_j(n) \tag{8}$$

$$y_{n+1} = p_{n+1} + h_n\, g_k(n)\, \phi_k(n+1) \tag{9}$$

where $h_n = x_{n+1} - x_n$

The coefficients are defined recursively:

$$\beta_j(n) = \beta_{j-1}(n)\frac{x_{n+1} - x_{n-j+1}}{x_n - x_{n-j}} \quad \text{with} \quad \beta_0(n) = 1 \tag{10}$$

$$\phi_j(n) = \phi_{j-1}(n) - \beta_{j-1}(n-1)\phi_{j-1}(n-1) \quad \text{with} \quad \phi_0(n) = f_n \tag{11}$$

$$g_j(n) = c_{j,1}(x_{n+1}) \tag{12}$$

$$c_{j,q}(x_{n+1}) = c_{j-1,q}(x_{n+1}) - c_{j-1,q+1}(x_{n+1})\frac{h_n}{x_{n+1} - x_{n-j+1}} \quad \text{with} \quad c_{0,q}(x_{n+1}) = \frac{1}{q} \tag{13}$$

2 Implementation

Here, all this theory should be put into practice and implemented into the DynStar source code. The most important step is to derive the correct formulas. The two-step ABM method has been chosen because its formulas are the easiest to derive and implement, but the code can be extended to allow other ABM methods with more complicated formulas. For $k = 2$, the formulas are derived as follows:

$$p_{n+1} = y_n + h^+(g_0(n)\,\beta_0(n)\,\phi_0(n) + g_1(n)\,\beta_1(n)\,\phi_1(n))$$

$$\Rightarrow p_{n+1} = y_n + h^+\left(f_n + \frac{1}{2}\frac{h^+}{h^-}(f_n - f_{n-1})\right) \tag{14}$$

$$\text{and} \quad y_{n+1} = p_{n+1} + h^+\,g_2(n)\,\phi_2(n+1)$$

$$\Rightarrow y_{n+1} = p_{n+1} + h^+\left(\frac{1}{2} - \frac{1}{6}\frac{h^+}{h^+ + h^-}\right)\left(f_{n+1} - f_n - \frac{h^+}{h^-}(f_n - f_{n-1})\right) \tag{15}$$

where $h^- = x_n - x_{n-1}$ is the previous stepsize and $h^+ = x_{n+1} - x_n$ is the following stepsize. Notice that if the stepsizes are equal, the formulas simplify to (6) and (7).

It's clear that the k-step ABM method needs information about k previous points in order to calculate the following value. However, in the beginning of the algorithm only one value is available: the initial condition $y(x_0) = y_0$. Hence the ABM method is not self-starting and another method is needed to calculate the k-1 first values. In our case, only one extra value is required and it is computed using one step of Runge-Kutta fourth order.

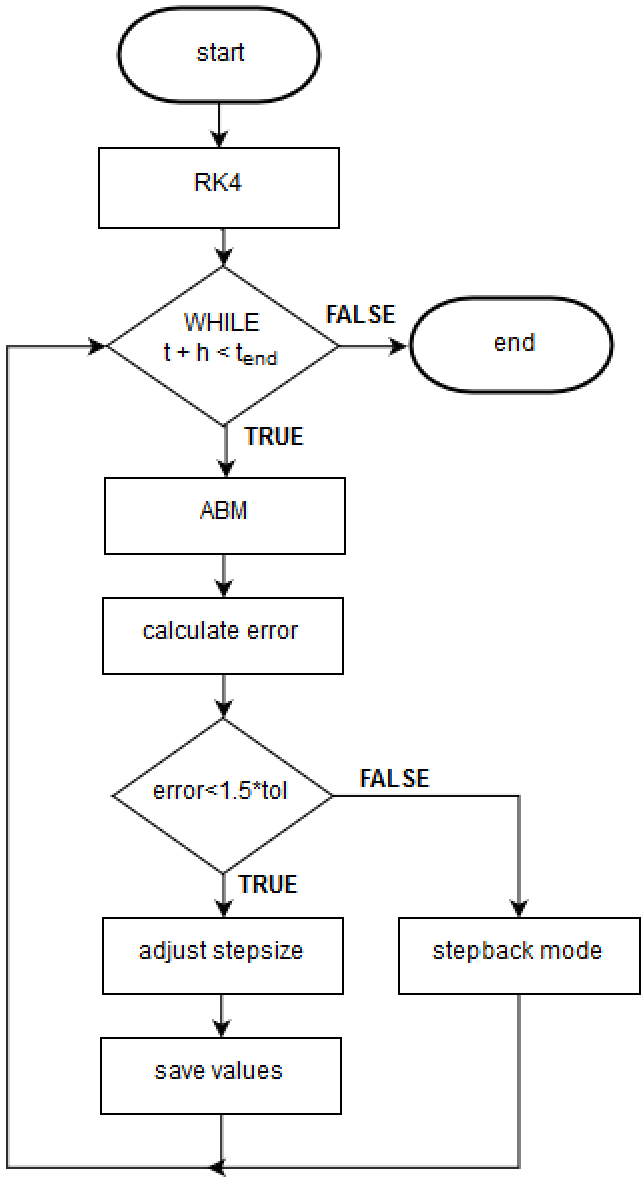
The next feature that needs to be implemented is the varying stepsize. The reasoning behind it is that the stepsize should always be small enough to ensure accurate results, yet large enough to avoid unnecessary calculations. The local truncation error can be used as a measure for accuracy. This error is estimated as the relative difference between the predicted and the corrected value.

$$\text{relative error} = \text{abs}\left(\frac{p_{n+1} - y_{n+1}}{y_{n+1}}\right) \tag{16}$$

When this error gets too large, i.e. when it exceeds a certain tolerance, the stepsize should be decreased immediately. On the other hand, when the error is below the tolerance, it is safe to increase the stepsize. With these properties in mind, Hanna [5] proposed a formula to adjust the stepsize:

$$h^+ = h^-\sqrt{\frac{tol}{rel}} \tag{17}$$

However, sometimes the error is unacceptably high, quantified by exceeding 1.5 times the tolerance. In this case, choosing a small stepsize for the following step is not enough; it is the stepsize for the current step that needs to be decreased. Then the program goes into a 'stepback mode', where none of the new values are saved and the current step is completely restarted with a smaller stepsize. The flowchart in Figure 1 shows how the algorithm is organized.



Source: Own

Fig. 1: *Flowchart of the algorithm*

3 Results

3.1 ABM Compared to RK4

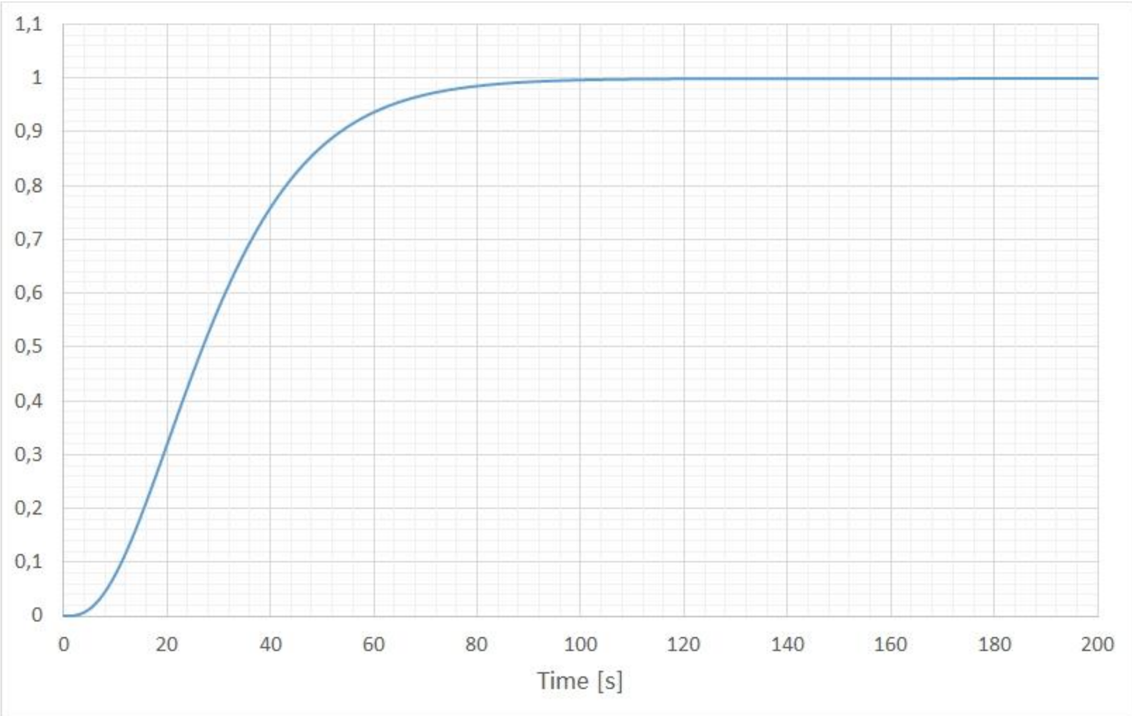
First, a comparison between ABM and RK4 is made. The methods are tested on a very simple third-order ordinary differential equation given by (18). The solution is shown in Figure 2.

$$y'_1 = \frac{1}{T_1}(u - y_1) \quad \text{with} \quad y_1(0) = 0$$

$$y'_2 = \frac{1}{T_2}(y_1 - y_2) \quad \text{with} \quad y_2(0) = 0 \tag{18}$$

$$y'_3 = \frac{1}{T_3}(y_2 - y_3) \quad \text{with} \quad y_3(0) = 0$$

$$t_0 = 0 \quad \text{and} \quad t_{end} = 200$$



Source: Own

Fig. 2: *Graph of PT3*

As ABM calculates only two function evaluations per integration step and RK4 calculates four, one would expect ABM to be twice as fast. However, in table 1 it can be seen that the results do not support this hypothesis. In fact, the amount of time needed by the two methods is approximately the same. The explanation is that the function evaluation is very simple or cheap and does not account for a large portion of the runtime. Therefore, it can almost be neglected whether the evaluation is done two or four times. But when the differential equation is computationally expensive, the amount of function evaluations will certainly be reflected in the runtime. To demonstrate this, we still use the same problem given by (18) but we make it expensive by adding a delay of 1ms. Now it is clear that Runge-Kutta takes twice as much time as ABM. In all tables, the time is expressed in seconds.

Tab. 1: *ABM compared to RK4*

TOL	Steps		Time (cheap evaluation)		Time (expensive evaluation)	
	ABM	RK4	ABM	RK4	ABM	RK4
10^{-4}	116	121	0.02	0.02	0.46	0.95
10^{-7}	1014	1037	0.14	0.15	3.99	8.12

Source: Own

3.2 ABM Compared to Hanna, Stiff Problem

The method that has already been implemented in DynStar is the one Hanna proposed in his paper [5]. It is important to understand which method is more effective for different cases, so that a DynStar user can choose the right option. Hanna method takes a weighted average of the values obtained by the Euler method and the RK2 (or improved Euler) method. The great advantage of the Hanna method is that it has a large stability domain. For stiff problems the stepsize is limited rather for stability reasons than accuracy reasons. This means that a stable method such as Hanna will be able to take bigger steps, hence saving time. Unfortunately, ABM doesn't handle stiff problems very well and is more suitable for non-stiff problems. We will test this hypothesis on a mildly stiff problem, also discussed by Hanna in his paper, called Robertson chemical reaction system, given by (19). In Figures 3 and 4, the solution is shown for different end times. Both graphs are in linear scale.

$$y'_1 = -0.04 \cdot y_1 + 10^4 \cdot y_2 y_3 \quad \text{with} \quad y_1(0) = 1$$

$$y'_2 = 0.04 \cdot y_1 - 10^4 \cdot y_2 y_3 - 3 \cdot 10^7 {y_2}^2 \quad \text{with} \quad y_2(0) = 0 \tag{19}$$

$$y'_3 = 3 \cdot 10^7 {y_2}^2 \quad \text{with} \quad y_3(0) = 0$$

$$t_0 = 0 \quad \text{and} \quad t_{end} = 10$$

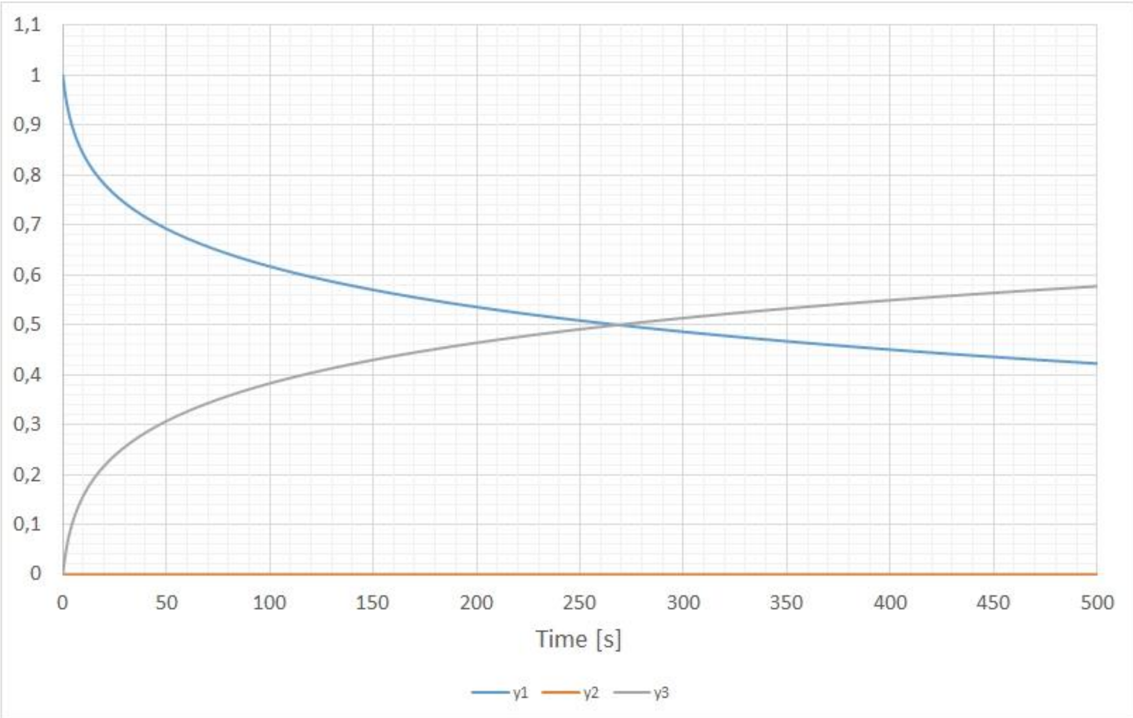


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Fig. 3: *Graph of Robertson chemical reaction system, t: 0 → 500 seconds*

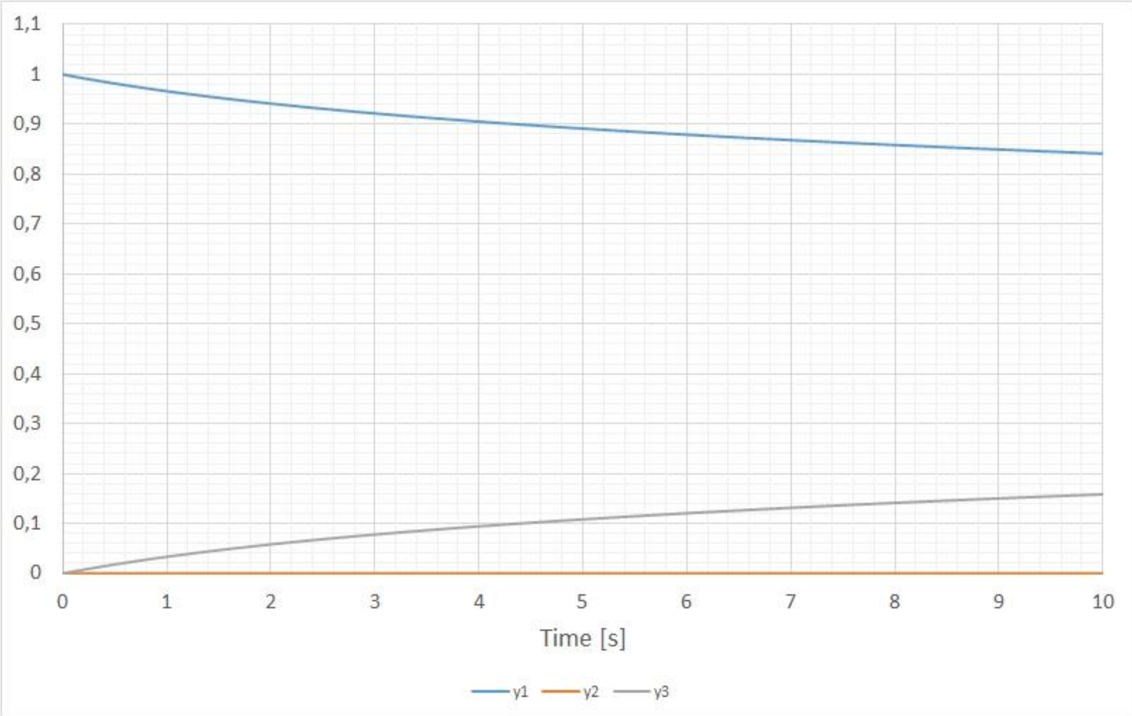

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Fig. 4: *Graph of Robertson chemical reaction system, t: 0 → 10 seconds*

The results in Table 2 show that ABM is forced to take small steps in order to maintain stability, while achieving high accuracy in the process. On the other hand, Hanna is much faster and in many cases this is preferred. Only when tolerances are very strict, Hanna gets in trouble because it cannot be used to obtain highly accurate results. In the following table, RE is the relative error between the computed solution for y_3 at $t = 10$ and the exact solution $y_3(10) = 0.1586138397$.

Tab. 2: *ABM compared to Hanna in case of a moderately stiff problem*

TOL	RE		Steps		Time	
	ABM	HAN	ABM	HAN	ABM	HAN
10^{-2}	$2.8 \cdot 10^{-6}$	$1.2 \cdot 10^{-4}$	13696	3931	1.34	0.28
10^{-3}	$3.4 \cdot 10^{-8}$	$1.8 \cdot 10^{-4}$	14022	4083	1.42	0.35
10^{-4}	$1.5 \cdot 10^{-8}$	$1.3 \cdot 10^{-4}$	14060	4550	1.37	0.37
10^{-5}	$1.6 \cdot 10^{-8}$	$1.2 \cdot 10^{-4}$	14159	5284	1.31	0.39
10^{-6}	$1.6 \cdot 10^{-8}$	$8.9 \cdot 10^{-5}$	14475	8597	1.43	0.81
10^{-7}	$1.6 \cdot 10^{-8}$	$5.8 \cdot 10^{-5}$	14753	19397	1.54	1.90
10^{-8}	$1.6 \cdot 10^{-8}$	$2.6 \cdot 10^{-5}$	15733	54924	1.71	4.92

Source: Own

3.3 ABM Compared to Hanna, Non-stiff Problem

Further, the performances of these two methods are compared for a non-stiff problem. We use a differential equation system similar to (18). The difference is that now we use a tenth order ODE given by (20) and all time constants are chosen to be equal, ensuring a non-stiff problem. The solution is shown in Figure 5.

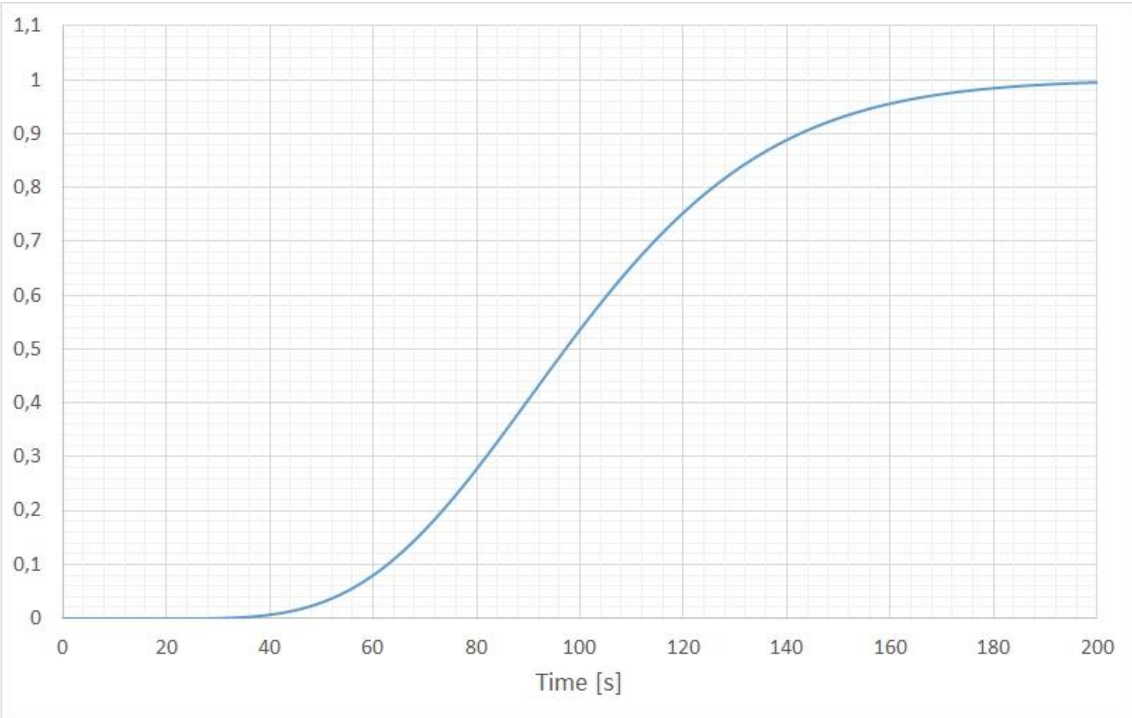
$$y'_1 = \frac{1}{T}(u - y_1) \quad \text{with} \quad y_1(0) = 0$$

$$y'_2 = \frac{1}{T}(y_1 - y_2) \quad \text{with} \quad y_2(0) = 0$$

$$\vdots \tag{20}$$

$$y'_{10} = \frac{1}{T}(y_9 - y_{10}) \quad \text{with} \quad y_{10}(0) = 0$$

$$t_0 = 0 \quad \text{and} \quad t_{end} = 200$$



Source: Own

Fig. 5: *Graph of PT10*

Now the results in table 3 are very positive for ABM because this method is both faster and more accurate than the Hanna method. This can be explained by remembering that for a non-stiff problem, stability is not much of an issue. This means that an accurate method such as ABM can allow for taking bigger steps than a stable method such as Hanna, hence needing fewer steps and less time. In table 3, RE is defined as the relative error between the computed solution for y_{10} at $t = 200$ and the exact solution $y_{10}(200) = 0.9947057955$.

Tab. 3: *ABM compared to Hanna in case of a non-stiff problem*

TOL	RE		Steps		Time	
	ABM	HAN	ABM	HAN	ABM	HAN
10^{-2}	$3.5 \cdot 10^{-3}$	$5.8 \cdot 10^{-3}$	1279	1621	0.12	0.17
10^{-3}	$3.8 \cdot 10^{-4}$	$3.0 \cdot 10^{-3}$	1623	2942	0.21	0.52
10^{-4}	$4.0 \cdot 10^{-5}$	$1.1 \cdot 10^{-3}$	2362	7120	0.39	1.46
10^{-5}	$4.0 \cdot 10^{-6}$	$3.8 \cdot 10^{-4}$	3954	20326	0.82	4.41
10^{-6}	$4.2 \cdot 10^{-7}$	$1.2 \cdot 10^{-4}$	7383	62087	1.68	14.39

Source: Own

Conclusion

The goal of the assignment was to improve the simulation tool DynStar by adding another solver algorithm for differential equations. After literature research, we succeeded to develop formulas for a multistep method with a variable stepsize, namely the two-step Adams-Bashforth-Moulton predictor-corrector method as described by Krogh. The method has been tested and the following conclusions can be drawn. ABM is most effective when function evaluations are expensive and/or when the problem is non-stiff. On the other hand, when function evaluations are cheap, ABM still presents good, but not significantly better results than RK4. In the case of a stiff problem, the Hanna method is more efficient in terms of runtime; however, the ABM method gets more accurate results. Altogether, we can conclude that the ABM algorithm is a valuable addition to the DynStar software and that it will prove itself useful by solving many differential equations more accurately and/or more efficiently than the methods that have already been implemented.

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ROZVOJ A REALIZACE DVOUKROKOVÉ ADAMS-BASHFORTH-MOULTONOVY METODY S VARIABILNÍ VELIKOSTÍ KROKŮ U SIMULAČNÍHO NÁSTROJE DYNSTAR

Simulační nástroj DynStar, vytvořený na katedře IPM na Hochschule Zittau / Görlitz, dříve používal pro řešení diferenciálních rovnic pouze jednokrokové metody. Tento článek popisuje vývoj vícekrokové metody doplňující ostatní metody. Úvodní část dává čtenáři lepší představu o užitečnosti vícekrokové metody. Teoretická část je zaměřena na dvoukrokovou Adams-Bashforth-Moultonovu metodu (ABM), a možnost vhodného využití vzorců pro variabilní velikost kroků (stepsize). Poté je vytvořen algoritmus řešení diferenciálních rovnic za použití vzorců ABM a úpravou stepsize podle odchylky mezi predikcí a korekcí. To je popsáno v sekci Realizace. V závěrečné sekci článku (Výsledky) je metoda ABM porovnána s metodami RK4 a Hanna.

ENTWICKLUNG UND IMPLEMENTIERUNG DES ZWEI-SCHRITT-ADAMS-BASHFORTH-MOULTON-VERFAHREN MIT VARIABLER SCHRITTWEITE FÜR DAS SIMULATIONSWERKZEUG DYNSTAR

Das Simulationswerkzeug DynStar, das von der Hochschule Zittau / Görlitz IPM entwickelt wird, verwendet bisher nur einstufige Methoden zur Lösung von Differentialgleichungen. Dieser Beitrag beschreibt die Entwicklung eines mehrstufigen Verfahrens. Die Einleitung gibt legt dar, warum eine mehrstufige Methode nützlich sein kann. Der Theorieteil konzentriert sich auf das zweistufige Adams-Bashforth-Moulton (ABM)-Verfahren und wie es für variable Schrittweiten angepasst wurde. Es wurde ein Algorithmus entwickelt, um die Differentialgleichungen unter Verwendung des ABM-Methode zu lösen und die Schrittweite entsprechend dem Fehler zwischen der Vorhersage und der Korrektur zu bestimmen. Dies wird im Implementierungsabschnitt beschrieben. Abschließend wird die ABM-Methode mit dem Runge-Kutta-Verfahren 4. Ordnung und der Hanna-Methode im Ergebnisabschnitt verglichen.

OPRACOWANIE I REALIZACJA DWUKROKOWEJ METODY ADAMS-BASHFORTH-MOULTONA ZE ZMIENNĄ WIELKOŚCIĄ KROKÓW W NARZĘDZIU SYMULACYJNYM DYNSTAR

Narzędzie symulacyjne DynStar, opracowane w katedrze IPM (procesów automatyzacyjnych i technik pomiarowych) w Hochschule Zittau/Görlitz, do rozwiązywania równań różniczkowych wykorzystywało dawniej wyłącznie metody jednokrokowe. W niniejszym artykule opisano proces opracowania metody kilkukrokowej będącej uzupełnieniem innych metod. W pierwszej części przedstawiono zalety metody kilkukrokowej. W części teoretycznej skupiono się na dwukrokowej metodzie Adams-Bashforth-Moultonaa (ABM) oraz możliwości odpowiedniego wykorzystania wzorów do zmiennej wielkości kroków (stepsize). Następnie opracowano algorytm służący rozwiązywaniu równań różniczkowych z zastosowaniem wzorów ABM i dostosowaniem stepsize w zależności od odchylenia pomiędzy prognozą a korektą. Opisano to w części Realizacja. W końcowej części artykułu (Výsledky - Wyniki) metodę ABM porównano z metodami RK4 i Hanna.

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